Flow equations for Hamiltonians: Contrasting different approaches by using a numerically solvable model

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To contrast different generators for flow equations for Hamiltonians and to discuss the dependence of physical quantities on unitarily equivalent, but effectively different initial Hamiltonians, a numerically solvable model is considered which is structurally similar to impurity models. By this we discuss the question of optimization for the first time. A general truncation scheme is established that produces good results for the Hamiltonian flow as well as for the operator flow. Nevertheless, it is also pointed out that a systematic and feasible scheme for the operator flow on the operator level is missing. For this, an explicit analysis of the operator flow is given for the first time. We observe that truncation of the series of the observable flow after the linear or bilinear terms does not yield satisfactory results for the entire parameter regime as - especially close to resonances - even high orders of the exact series expansion carry considerable weight.

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I. INTRODUCTION

A. Flow equations

Eight years ago, Głazek and Wilson[1] and independently Wegner[2] introduced a new non-perturbative method to diagonalize, renormalize or simplify a given Hamiltonian. Whereas in high energy physics the method is known as "similarity transformations", the term "flow equations" has been established in the solid-state community. The idea is conceptually simple: Instead of diagonalizing the Hamiltonian of the system by a single unitary transformation, one performs a continuous sequence of infinitesimal unitary transformations and thus induces a flow on the system parameters. The procedure is not constrained to specific symmetries nor to certain parameter regimes - but is accessible to any system described by a Hamiltonian. Thus, the method has been successfully applied to various models of solid-state and nuclear physics. Examples are dissipative quantum systems[3,4,5], the electron-phonon problem[6,7] or the Hubbard model[8]. For a recent review on the flow equation method see Ref. 9.

The main advantage of the method is its flexibility. This is similar to the numerical diagonalization of a given matrix: There are many different possibilities to reach the goal. One is free to choose the basis in which the diagonalization is performed and within a given basis one is free to choose the concrete series of unitary transformations that finally diagonalizes the matrix. Depending on the basis and on the concrete series of unitary transformations, convergence may be good or poor, numerical errors may be small or large.

Similarly, many different flow equations can be formulated to diagonalize or simplify a given Hamiltonian. Even though all different flow equations are equivalent and will eventually lead to the same result, matters change as soon as approximations are involved. Typically one needs to cut the hierarchy of newly generated interaction terms and then neglect operators, which are assumed to be *irrelevant*. Yet, there is no satisfactory definition for *irrelevant operators* within the flow equation approach. Whether or not a contribution is irrelevant depends on the initial Hamiltonian and on the goal on wants to reach.

Usually, approximations were justified when certain sum rules, mostly stemming from the invariance of commutation relations during the unitary flow, hold exactly or at least asymptotically[5,7]. In addition, exact relations between static and dynamic properties - as the generalized Shiba relation in the case of the spin-boson model[10] - can serve as justification for prior approximations[5]. A general consistency check lies in the explicit investigation of the flow of the neglected operators.

So far, a detailed discussion on optimization of flow equations is missing. With this work, we want to start to fill this gap by addressing the following questions: E.g., any initial Hamiltonian H implicitly depends on a number of parameters $H = H(\psi, \theta, ...)$ where the parameters are associated to certain unitary transformations $U_1(\psi)$, $U_2(\theta)$, ... Can the parameters ψ, θ, ... be chosen such that a given flow equation scheme yields optimal results? A second variation that will be discussed lies in the arbitrary definition of the "diagonal" Hamiltonian, H_0 - as mentioned above. Will different H_0 yield similar results for physical quantities and is there an optimal H_0 for all physical quantities - or does the optimal H_0 depend on the physical quantity under scrutiny?

Another fundamental question associated with the flow equation approach is connected to the observable flow and

has not been discussed in depth yet, either. For this, we note that in order to take advantage of the simple structure of the fixed point Hamiltonian, the observable has to be transformed as well - by the same sequence of unitary transformations that diagonalized the Hamiltonian. Since usually the continuous transformation is designed such that the diagonalization of the Hamiltonian is "optimal", the observable flow is more likely to suffer from uncontrolled approximations. We will address the question if there is a scheme that optimizes both, Hamiltonian and observable flow and also compare the observable flow on the operator level.

To do so, we will not proceed systematically but we will address these questions more specifically. Namely, we will consider an explicit model which is structurally similar to dissipative impurity models - but still exactly solvable via numerical diagonalization. We will call this model the Rabi model and it is presented in the next subsection. We use this model to test different approximation schemes and compare the results with the numerically exact solution. This strategy was first pursued by Richter in his diploma work[11]. We extend his work in various directions. One point is to investigate Hamiltonians where the reflection symmetry is broken. This is important if one wants to understand the mechanism of phase transition as being observed in the spin-boson model[12].

In Sec. II, we develop a general truncation scheme which yields good results over a wide range of the parameter space. Furthermore, we present a particular truncation scheme which leaves the Hamiltonian form-invariant during the flow. The question of the invariance of the flow equations with respect to the particular choice of initial Hamiltonians, provided that they only vary by a unitary transformation, is discussed. As a criterion for the quality of the flow equations, we look at the ground-state energy as function of the bias as an example for the flow of a parameter of the Hamiltonian. In Sec. III, we give a thorough discussion about the flow of observables. As reference we will not only investigate the expectation value of observables, but also compare the flow equation result with the exact solution *on the operator level* for the first time. For this, an expansion of the operator into a basis of normal ordered bosonic operators is given. In Sec. IV, we close with general remarks and conclusions.

B. The Rabi Hamiltonian

The specific model we use for our discussion of various realizations of flow equations and various approximation schemes is the spin-boson Hamiltonian with only one mode, which we will call the Rabi model in order to distinguish it from the spin-boson model with an arbitrary number of modes. The Hamiltonian is given by

$$H = -\frac{\Delta_0}{2}\sigma_x + \frac{\epsilon_0}{2}\sigma_z + \omega_0 b^\dagger b + \sigma_z \frac{\lambda_0}{2}(b + b^\dagger) + E_0 \quad . \tag{1}$$

Here, $b^{(\dagger)}$ denotes the bosonic degree of freedom and σ_i with $i = x, y, z$ are the Pauli spin matrices. They obey the canonical commutation relation $[b, b^\dagger] = 1$ and the spin-1/2 algebra $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$. Since there is only one mode present, a numerical diagonalization is feasible by truncating the bosonic Hilbert space after n bosonic excitations with some fixed value of n.

The model was first introduced in the context of spontaneous emission and absorption of atoms and due to its long history there exists an enormous amount of work that has already been published on this model. It is impossible to review or cite all these papers - a good overview may be found in the paper by Graham *et al*[13]. The model has also been discussed in connection with quantum chaos[14,15] and extensions of it can serve for the description of optical phonons interacting with two-level systems or quantum dots within a solid-state matrix[16]. In the context of flow equations, the model has been discussed by Mielke[17] using a set of flow equations that preserve the banded structure of the Hamiltonian. In the present work we focus on low energy properties of the Rabi model. Ref. 17 is in some sense complementary to the present work since there the high energy modes were discussed.

In the present work we are interested in general properties of the flow equation method. The reasons for us to investigate the Rabi model lie in the fact that it couples a two-level system to a "bath" resembled by the bosonic degree of freedom. And since we only consider one mode, the system is still exactly solvable via numerical diagonalization.

II. FLOW OF THE HAMILTONIAN

A. Setting up the basis

In order to diagonalize the Hamiltonian (1), we will perform a continuous unitary transformation. The flow equations are generated by the anti-hermitian operator η which is canonically given by $\eta = [H_0, H]$, where H_0 defines the diagonal Hamiltonian[2]. Different choices of η are possible as well. The flow equations are of the form

$$\frac{dH}{d\ell} = [\eta, H] \quad , \tag{2}$$

where both H and η depend on the flow parameter ℓ. The choice $\eta = [H_0, H]$ is likely to decouple the fermionic system from the bosonic system, and the fixed point Hamiltonian $H(\ell = \infty)$ is then basically given by H_0^* where the asterisk indicates that the parameters of the initial diagonal Hamiltonian are in general renormalized. For a brief introduction, we refer to Appendix A, which treats the Rabi model with $\Delta = 0$ and motivates the approach given here.

Obviously, different choices for H_0 can lead to different flow equations. Another ambiguity stems from the fact that the initial Hamiltonian may differ by a unitary transformation. If we restrict ourselves to orthogonal transformations in the two-dimensional Hilbert space and to simple translations in the bosonic Hilbert space, i.e.

$$U_S = \begin{pmatrix} \cos\frac{\psi}{2} & \sin\frac{\psi}{2} \\ -\sin\frac{\psi}{2} & \cos\frac{\psi}{2} \end{pmatrix} \quad , \quad U_B = \exp(\theta\frac{\lambda_0}{2\omega_0}(b - b^\dagger)) \quad , \tag{3}$$

the general initial Hamiltonian with respect to the Hamiltonian (1) is given by

$$H = -\frac{\Delta'}{2}\sigma_x + \frac{\epsilon'}{2}\sigma_z + \omega_0 b^\dagger b + \frac{\lambda^e}{2}(b + b^\dagger) + \sigma_x\frac{\lambda^x}{2}(b + b^\dagger) + \sigma_z\frac{\lambda^z}{2}(b + b^\dagger) + E' \quad , \tag{4}$$

where we introduced the following parameters:

$$\Delta' = \Delta_0 \cos\psi + \tilde{\epsilon}\sin\psi \quad , \quad \epsilon' = \tilde{\epsilon}\cos\psi - \Delta_0\sin\psi \tag{5}$$

$$\lambda^e = \theta\lambda_0 \quad , \quad \lambda^x = -\sin\psi\lambda_0 \quad , \quad \lambda^z = \cos\psi\lambda_0 \tag{6}$$

$$E_0' = E_0 + \theta^2\frac{\lambda_0^2}{4\omega_0} \quad , \quad \tilde{\epsilon} = \epsilon_0 + \theta\frac{\lambda_0^2}{\omega_0} \tag{7}$$

As was mentioned above, different generators and different unitarily equivalent Hamiltonians will lead to the same physical results if no approximations are involved. But the above model is not solvable analytically and therefore approximations become necessary. In the special case of the Rabi model the flow equations will generate an infinite series of new coupling terms which cannot be summed up formally to yield a closed expression[18].

In this section we will first only take coupling terms into account which are linear in the bosonic operators and have real coefficients. This means that with respect to the initial Hamiltonian (4), only the term $i\sigma_y(b - b^\dagger)$ will be newly generated which resembles the lowest order of the polaron transformation (see e.g. Ref. 12). Using a generator which is not of the simple form $\eta = [H_0, H]$, we will also discuss flow equations which leave the initial Hamiltonian form-invariant. We are able to show analytically that the fixed point of the flow equation is independent with respect to the (distinguished) unitary transformation.

B. Flow equations with respect to the Canonical Generator

In the following subsection we will discuss flow equations which are obtained by employing the canonical generator $\eta = [H_0, H]$. This gives rise to new interaction terms. The truncated Hamiltonian shall be given by

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b + \frac{\lambda^e}{2}(b + b^\dagger) + \sigma_x\frac{\lambda^x}{2}(b + b^\dagger) + i\sigma_y\frac{\lambda^y}{2}(b - b^\dagger) + \sigma_z\frac{\lambda^z}{2}(b + b^\dagger) + E \quad , \tag{8}$$

where all parameters but the bath energy ω_0 are explicitly ℓ-dependent. The above Hamiltonian represents the most general Hermitian operator which includes all possible interaction terms acting on the underlying Hilbert space up to linear bosonic operators with real coefficients.

The flow shall be governed by the generator

$$\eta = i\sigma_y\eta^{0,y} + \eta^e(b - b^\dagger) + \sigma_x\eta^x(b - b^\dagger) + i\sigma_y\eta^y(b + b^\dagger) + \sigma_z\eta^z(b - b^\dagger) \tag{9}$$
$$\equiv \hat{\eta}^{0,y} + \hat{\eta}^e + \hat{\eta}^x + \hat{\eta}^y + \hat{\eta}^z \quad ,$$

where the parameters $\eta^{0,y}$, η^e, η^x, η^y, and η^z are ℓ-dependent and will be specified later.

The above generator represents the most general anti-Hermitian operator which includes all possible operators acting on the underlying Hilbert space up to linear bosonic operators with real coefficients.

1. Setting up the flow equations

The commutator $[\eta, H]$ yields the following contributions:

$$[\hat{\eta}^{0,y}, H] = -\sigma_z \Delta \eta^{0,y} - \sigma_x \epsilon \eta^{0,y} + \sigma_z \eta^{0,y} \lambda^x (b + b^\dagger) - \sigma_x \eta^{0,y} \lambda^z (b + b^\dagger) \tag{10}$$

$$[\hat{\eta}^e, H] = \eta^e \omega_0 (b + b^\dagger) + \eta^e \lambda^e + \sigma_x \eta^e \lambda^x + \sigma_z \eta^e \lambda^z \tag{11}$$

$$[\hat{\eta}^x, H] = -i\sigma_y \epsilon \eta^x (b - b^\dagger) + \sigma_x \eta^x \omega_0 (b + b^\dagger)$$
$$+ \sigma_x \eta^x \lambda^e + \eta^x \lambda^x - \sigma_z \eta^x \lambda^y (b - b^\dagger)^2 - i\sigma_y \eta^x \frac{\lambda^z}{2} \{(b - b^\dagger), (b + b^\dagger)\} \tag{12}$$

$$[\hat{\eta}^y, H] = -\sigma_z \Delta \eta^y (b + b^\dagger) - \sigma_x \epsilon \eta^y (b + b^\dagger) + i\sigma_y \eta^y \omega_0 (b - b^\dagger)$$
$$+ \sigma_z \eta^y \lambda^x (b + b^\dagger)^2 + \eta^y \lambda^y - \sigma_x \eta^y \lambda^z (b + b^\dagger)^2 \tag{13}$$

$$[\hat{\eta}^z, H] = -i\sigma_y \Delta \eta^z (b - b^\dagger) + \sigma_z \eta^z \omega_0 (b + b^\dagger) + \sigma_z \eta^z \lambda^e$$
$$+ i\sigma_y \eta^z \frac{\lambda^x}{2} \{(b - b^\dagger), (b + b^\dagger)\} + \sigma_x \eta^z \lambda^y (b - b^\dagger)^2 + \eta^z \lambda^z \tag{14}$$

$\{.,.\}$ denotes the anti-commutator. As can be seen in (12) - (14), the flow equations generate terms which are bilinear in the bosonic operators and we will need to find a suitable procedure how to include these terms in the flow. Kehrein, Mielke, and Neu[3] proposed to neglect these terms after normal ordering them with respect to a bilinear bosonic Hamiltonian. Since we allow the initial Hamiltonian to differ by a shift in the bosonic operators, we need to include this generalization also in the normal ordering procedure, i.e. we will normal order with respect to the shifted bosonic mode

$$\bar{b} \equiv b + \frac{\delta}{2} \quad, \tag{15}$$

with the linear shift δ to be determined later. To close the flow equations we will thus neglect the normal ordered operators

$$\mathcal{O}_1 = -\sigma_x \eta^y \lambda^z : (\bar{b} + \bar{b}^\dagger)^2 : \quad , \quad \mathcal{O}_2 = \sigma_z \eta^y \lambda^x : (\bar{b} + \bar{b}^\dagger)^2 : \quad , \tag{16}$$

$$\mathcal{O}_3 = \sigma_x \eta^z \lambda^y : (\bar{b} - \bar{b}^\dagger)^2 : \quad , \quad \mathcal{O}_4 = -\sigma_z \eta^x \lambda^y : (\bar{b} - \bar{b}^\dagger)^2 : \quad , \tag{17}$$

$$\mathcal{O}_5 = i\sigma_y (\eta^z \frac{\lambda^x}{2} - \eta^x \frac{\lambda^z}{2}) : \{(\bar{b} - \bar{b}^\dagger), (\bar{b} + \bar{b}^\dagger)\} : \quad . \tag{18}$$

Normal ordering is now defined as $: (\bar{b} + \bar{b}^\dagger)^2 := (\bar{b} + \bar{b}^\dagger)^2 - 1_n$, with $1_n \equiv \langle (\bar{b} + \bar{b}^\dagger)^2 \rangle = 1 + 2n$, and $n = (e^{\beta \omega_0} - 1)^{-1}$ being the Bose factor. Notice that the temperature enters in the Hamiltonian flow through normal ordering. In the following we will only consider $T = 0$, i.e. $1_n = 1$, but we will nevertheless keep track of this distinction.

Like in the case of flow equations for impurity systems[5], the above truncation scheme has the effect that the bosonic energy ω_0 is not being renormalized during the flow.

With $\frac{dH}{d\ell} = [\eta, H]$ we obtain the following flow equations:

$$\partial_\ell \Delta = 2\epsilon \eta^{0,y} - 2\eta^e \lambda^x - 2\eta^x \lambda^e + 2(\eta^z \lambda^y + \eta^y \lambda^z) 1_n - 2\eta^y \lambda^z \delta^2 \tag{19}$$

$$\partial_\ell \epsilon = -2\Delta \eta^{0,y} + 2\eta^z \lambda^e + 2(\eta^y \lambda^x + \eta^x \lambda^y) 1_n + 2\eta^e \lambda^z - 2\eta^y \lambda^x \delta^2 \quad , \quad \partial_\ell \lambda^e = 2\eta^e \omega_0 \tag{20}$$

$$\partial_\ell \lambda^x = -2\epsilon \eta^y + 2\eta^x \omega_0 - 2\eta^{0,y} \lambda^z + 4\eta^y \lambda^z \delta \quad , \quad \partial_\ell \lambda^y = -2\Delta \eta^z - 2\epsilon \eta^x + 2\eta^y \omega_0 - 2\eta^z \lambda^x \delta + 2\eta^x \lambda^z \delta \tag{21}$$

$$\partial_\ell \lambda^z = -2\Delta \eta^y + 2\eta^z \omega_0 + 2\eta^{0,y} \lambda^x - 4\eta^y \lambda^x \delta \quad , \quad \partial_\ell E = \eta^e \lambda^e + \eta^x \lambda^x + \eta^y \lambda^y + \eta^z \lambda^z \tag{22}$$

With $\lambda^e = \eta^e = 0$, an obvious invariant is given by $\mathrm{Inv} = \Delta^2 + \epsilon^2 + \lambda^{x2} + \lambda^{y2} + \lambda^{z2} - 4E\omega_0$. To investigate the flow equations further, one has to specify the constants and initial conditions. To do so we will choose different diagonal Hamiltonians H_0, and we will contrast the resulting flow equations by means of the ground-state energy of the system.

2. Determining the Canonical Generator

An obvious choice for the diagonal Hamiltonian is given by $H_0 = -\frac{\Delta}{2}\sigma_x + \omega_0 b^\dagger b$. The canonical generator $\eta = [H_0, H]$ is of the form (9) with $\eta^{0,y} = \Delta \epsilon/2$, $\eta^e = -\omega_0 \lambda^e/2$, $\eta^x = -\omega_0 \lambda^x/2$, $\eta^y = (\Delta \lambda^z - \omega_0 \lambda^y)/2$ and $\eta^z = (-\omega_0 \lambda^z + \Delta \lambda^y)/2$. We will refer to the flow equations with this particular choice of η as Version a.

Another choice for the diagonal Hamiltonian is given by $H_0 = \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b$. The canonical generator $\eta = [H_0, H]$ is of the form (9) with $\eta^{0,y} = -\Delta\epsilon/2$, $\eta^e = -\omega_0\lambda^e/2$, $\eta^x = (-\omega_0\lambda^x + \epsilon\lambda^y)/2$, $\eta^y = (\epsilon\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = -\omega_0\lambda^z/2$. We will refer to the flow equations with this particular choice of η as Version b.

The third choice for the generator which we will investigate in the following combines the two previous choices, i.e $\eta = [H_0, H]$ with $H_0 = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b$. The canonical generator η is of the form (9) with $\eta^{0,y} = 0$, $\eta^e = -\omega_0\lambda^e/2$, $\eta^x = (-\omega_0\lambda^x + \epsilon\lambda^y)/2$, $\eta^y = (\Delta\lambda^z + \epsilon\lambda^x - \omega_0\lambda^y)/2$ and $\eta^z = (-\omega_0\lambda^z + \Delta\lambda^y)/2$. We will refer to the flow equations with this particular choice of η as Version c.

There are other possibilities for the diagonal Hamiltonian which include coupling terms. We could e.g. choose $H_0 = \omega_0 b^\dagger b + \sigma_z \frac{\lambda^z}{2}(b + b^\dagger)$, since this Hamiltonian is also exactly solvable, see Appendix A. Another possibility is to choose the Jaynes-Cummings Hamiltonian as H_0[19] (see also Appendix D), which was done by Richter[11]. In this work though, we want to confine ourselves to the versions given above.

3. Determining the Bosonic Shift

We now want to determine the newly introduced bosonic shift δ. The procedure is not unambiguous, but we are led by formally diagonalizing the Hamiltonian as follows:

$$H = -\frac{\Delta'}{2}\sigma_x + \frac{\epsilon'}{2}\sigma_z + \omega_0\left(b^\dagger + \sum_j \sigma_j \frac{\lambda^j}{2\omega_0} + i\sigma_y \frac{\lambda^y}{2\omega_0}\right)\left(b + \sum_j \sigma_j \frac{\lambda^j}{2\omega_0} - i\sigma_y \frac{\lambda^y}{2\omega_0}\right) + E' \quad , \tag{23}$$

with $\Delta' \equiv \Delta + \frac{\lambda^e\lambda^x}{\omega} - \frac{\lambda^y\lambda^z}{\omega}$, $\epsilon' \equiv \epsilon - \frac{\lambda^e\lambda^z}{\omega} - \frac{\lambda^x\lambda^y}{\omega}$, and $E' \equiv E - \frac{\lambda^i\lambda^i}{4\omega} - \frac{\lambda^y\lambda^y}{4\omega}$ and summation is over $j = e, x, z$ with $\sigma_e \equiv 1$. Decoupling the fermionic and bosonic Hilbert space, we thus obtain the ℓ-dependent shift

$$\delta = \sum_j \langle\sigma_j\rangle \frac{\lambda^j}{\omega_0} \quad . \tag{24}$$

The fermionic expectation values can be evaluated directly with respect to the effective Hamiltonian $H^p = -\frac{\Delta'}{2}\sigma_x + \frac{\epsilon'}{2}\sigma_z$ to yield

$$\langle\sigma_x\rangle = \Delta'/R' \quad , \quad \langle\sigma_z\rangle = -\epsilon'/R' \quad , \quad \text{with } R'^2 \equiv \Delta'^2 + \epsilon'^2. \tag{25}$$

There is also a self-consistent possibility to determine the system expectation values. For that we will formulated the Hamiltonian with respect to the shifted mode $\bar{b} = b + \delta/2$. The renormalized "one-particle" parameters are then given by

$$\bar{\Delta} \equiv \Delta + \lambda^x\delta \quad , \quad \bar{\epsilon} \equiv \epsilon - \lambda^z\delta \quad . \tag{26}$$

Evaluating the system parameters now with respect to the system Hamiltonian $H^p = -\frac{\bar{\Delta}}{2}\sigma_x + \frac{\bar{\epsilon}}{2}\sigma_z$ and still assuming the bosonic shift as given in Eq. (24), we obtain the following self-consistent equations:

$$\langle\sigma_x\rangle = \bar{\Delta}/\bar{R} \quad , \quad \langle\sigma_z\rangle = -\bar{\epsilon}/\bar{R} \quad , \quad \text{with } \bar{R}^2 \equiv \bar{\Delta}^2 + \bar{\epsilon}^2 \quad . \tag{27}$$

In this work, we will restrict our investigation to the bosonic shift of (24) and to these two procedures of determining the fermionic expectation values. But there are other possibilities of evaluating the bosonic shift or the expectation values. One way is e.g. to couple the flow of the system parameters with the flow of the observable by imposing that a certain sum rule holds *exactly* (see next section). This condition will determine the bosonic shift. In the next section we show that the sum rule for the x- and z-component of the Pauli matrices is quadratic in the bosonic shift. But since we restricted ourselves to real shifts, there might be no solution. Even if we allowed imaginary coefficients in the evolution of the Hamiltonian, a solution would not be guaranteed since the sum rule would then relate the complex shift δ with its complex conjugate δ^*. Numerical investigations indicated that the bosonic shift δ cannot be chosen such that a certain sum rule holds exactly. It is left open, how this effects the stability and reliability of the flow equation approach.

Finally, we want to point out that the procedure of determining the expectation values can significantly alter the behavior of the flow equations. In case of the spin-boson model it is shown[20], that an infinitesimal bias resembles a relevant perturbation, i.e. $\partial_\ell\epsilon \propto \epsilon$ for small ℓ, if one chooses the expectation values directly whereas it resembles a irrelevant perturbation ($\partial_\ell\epsilon \propto -\epsilon$) if one chooses the self-consistent scheme.
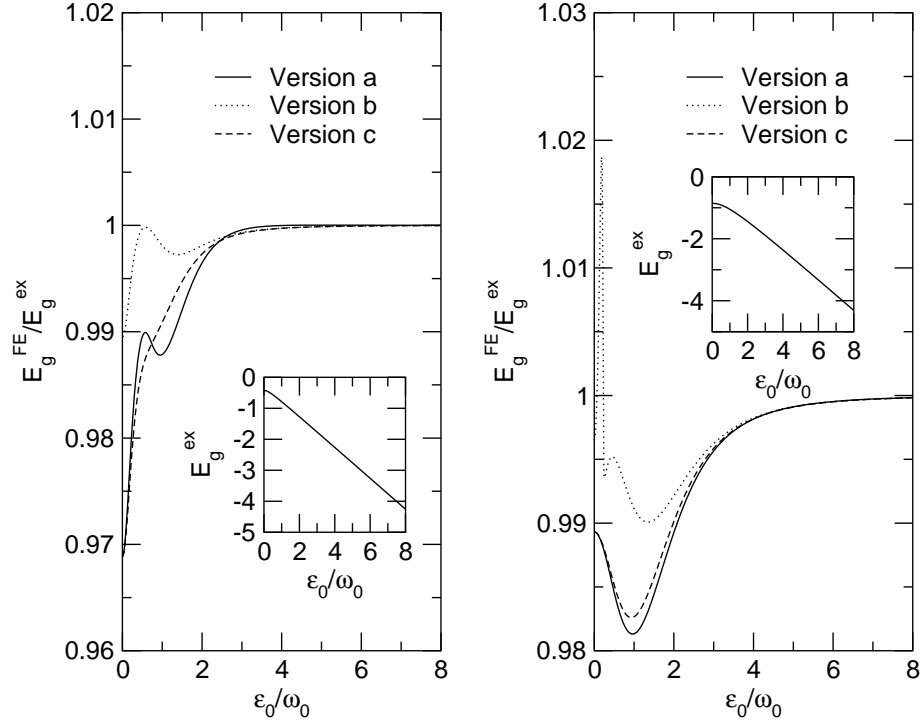
FIG. 1: The ground-state energy E_g^{FE} obtained by different canonical generators with $\psi = 0$ and $\theta = 0$ for $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel. The bosonic shift is set zero throughout the flow, i.e. $\delta = 0$ for all ℓ.

4. Numerical Results

We want to analyze the quality of the above flow equations by means of the ground-state energy E_g of the system as a function of the external bias ϵ_0. These results are compared with the numerically exact solution obtained via numerical diagonalization. Since the bosonic mode is left un-renormalized, the energy scale is given by ω_0. For the coupling constant we choose $\lambda_0 = \omega_0$, i.e. we are not in the perturbative regime.

We will first consider the flow of the initial Hamiltonian with $\theta = 0$ and $\psi = 0$. We will also set $\delta = 0$ for all ℓ. In Fig. 1 the ground-state energies E_g^{FE} obtained from the different canonical generators are shown. Calculations are done for two different tunnel-matrix elements $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ (right hand side), the first below and the second above resonance. Resonance in the un-perturbed system is defined by $\Delta_0/\omega_0 = 1$. All results are in good agreement with the numerically exact solution. Still, differences occur in the non-trivial regime where the bias ϵ_0 is below or around the energy scale given by ω_0. In the panels, the exact ground-state energies E_g^{ex} are displayed.

We now turn to the flow equations obtained by employing the generalized normal ordering procedure, i.e. we set $\delta = \sum_j \langle \sigma_j \rangle \lambda^j / \omega_0$. The results for the different generators are shown in Fig. 2. The expectation values are determined directly according to Eqs. (25) (left hand side) and self-consistently according to Eqs. (27) (right hand side). There is a systematic improvement to the results of Fig. 1, where δ was set zero for all ℓ. The best results are obtained by the generator of Version b and determining the expectation values self-consistently.

Finally, we want to investigate the dependence of the flow equations on the unitarily equivalent, but different representations of the initial Hamiltonian, labeled by ψ and θ. For this we choose the generator of Version b and the bosonic shift of (24) with the direct evaluation of the expectation values according to Eqs. (25). On the left hand side of Fig. 3 we vary ψ with $\theta = 0$; on the right hand side of Fig. 3 we vary θ with $\psi = 0$.

As can be seen, there are differences with respect to the initial Hamiltonian. For $\psi = \pi/4$, there is a big deviation from the exact value in a small region around $\epsilon_0 \approx 1.5$ with a maximum of 1.2. In this region the fixed point Hamiltonian $H(\ell = \infty)$ varies from the "normal" fixed point Hamiltonian and the ground-state energy is mostly determined by $E(\ell = \infty)$. This is also the case for $\theta \leq -1$ (not shown) where the regions of large deviations depend on θ. Still, we observe a certain invariance with respect to the initial Hamiltonian keeping the crude truncation scheme in mind.
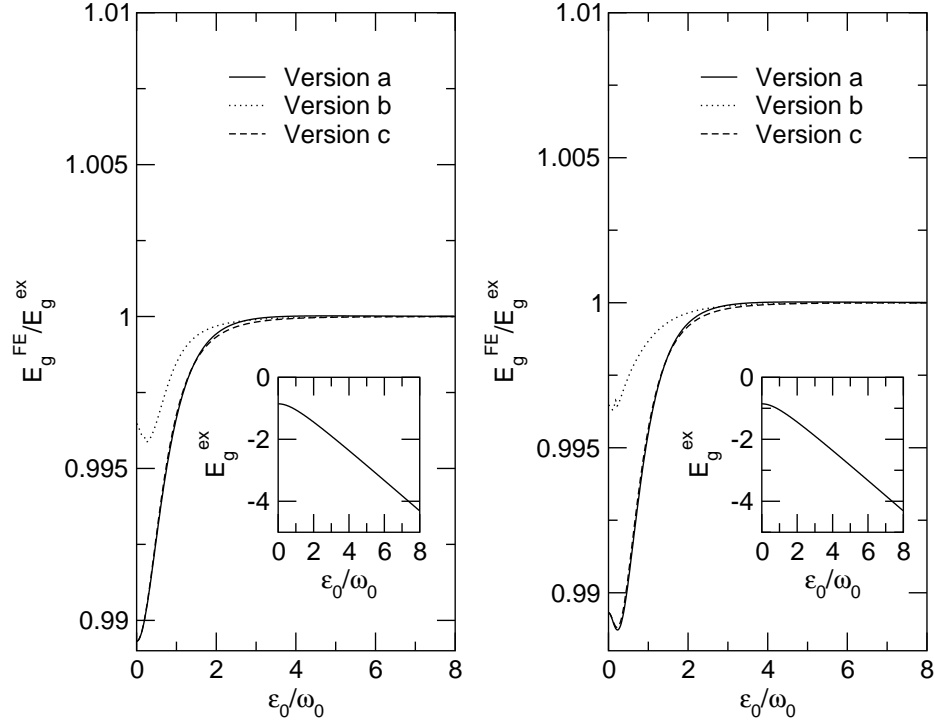
FIG. 2: The ground-state energy E_g^{FE} obtained by different canonical generators with $\psi = 0$ and $\theta = 0$ for $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel. The expectation values for the bosonic shift $\delta = \sum_j \langle \sigma_j \rangle \lambda^j / \omega_0$ were evaluated directly according to Eqs. (25) (left hand side) and self consistently according to Eqs. (27) (right hand side).

From the considered parameters, the best results are obtained for $\psi = 0$ and $\theta = -0.5$. Of course, it would be desirable to give an objective scheme how to choose the representation of the initial Hamiltonian that yields the best result for the ground-state energy. This had to be left open.

C. Flow equations with respect to a Form-Invariant Flow

As was mentioned above, the canonical generator $\eta = [H_0, H]$, in general, gives rise to new interaction terms. In order to avoid this complication, Kehrein, Mielke, and Neu pursued a different strategy to set up the flow equations, namely they chose the generator η such that the Hamiltonian remains form-invariant. To assure that the initial Hamiltonian of Eq. (1) remains form-invariant, we set $\delta = 0$, and the constants of the generator of Eq. 9 have to satisfy the following relations:

$$\eta^e = 0 \quad , \quad -\epsilon \eta^y + \eta^x \omega_0 - \eta^{0,y} \lambda^z = 0 \quad , \quad -\Delta \eta^z - \epsilon \eta^x + \eta^y \omega_0 = 0 \qquad (28)$$

This guarantees that λ^e, λ^x and λ^y are not being generated. With these relations, the parameters are defined up to a common factor f. If one chooses $\eta^z = -\omega_0 \lambda^z f/2$, one finds $\eta^{0,y} = \epsilon \Delta f/2$, $\eta^e = 0$, $\eta^x = 0$ and $\eta^y = -\Delta \lambda^z f/2$. With this choice, all neglected operators except of $\mathcal{O}_1$ vanish. One obtains the following coupled differential equations:

$$\partial_\ell \Delta = -\Delta \lambda^{z2} f 1_n + \Delta \epsilon^2 f \quad , \quad \partial_\ell \epsilon = -\epsilon \Delta^2 f$$
$$\partial_\ell \lambda^z = \lambda^z (\Delta^2 - \omega_0^2) f \quad , \quad \partial_\ell E = -\omega_0 \lambda^{z2} f/2 \qquad (29)$$

For the numerical calculations, we set $f = 1$ and refer to this set of flow equations as Version d.

We want to consider the form-invariant flow after having performed a unitary transformation on the two-dimensional Hilbert space which diagonalizes $H^p = -\frac{\Delta_0}{2}\sigma_x + \frac{\epsilon_0}{2}\sigma_z \rightarrow \frac{R}{2}\sigma_z$ with $R^2 = \Delta_0^2 + \epsilon_0^2$. This is achieved by choosing $\tan \psi = -\Delta_0/\epsilon_0$. If we thus want to avoid the generation of Δ, λ^e, and λ^y as defined in (8), we set $\delta = 0$, and the parameters of the generator have to satisfy the following conditions:

$$R \eta^{0,y} + \eta^y \lambda^z 1_n = 0 \quad , \quad \eta^e = 0 \quad , \quad -\Delta \eta^z - R \eta^x + \eta^y \omega_0 = 0 \qquad (30)$$
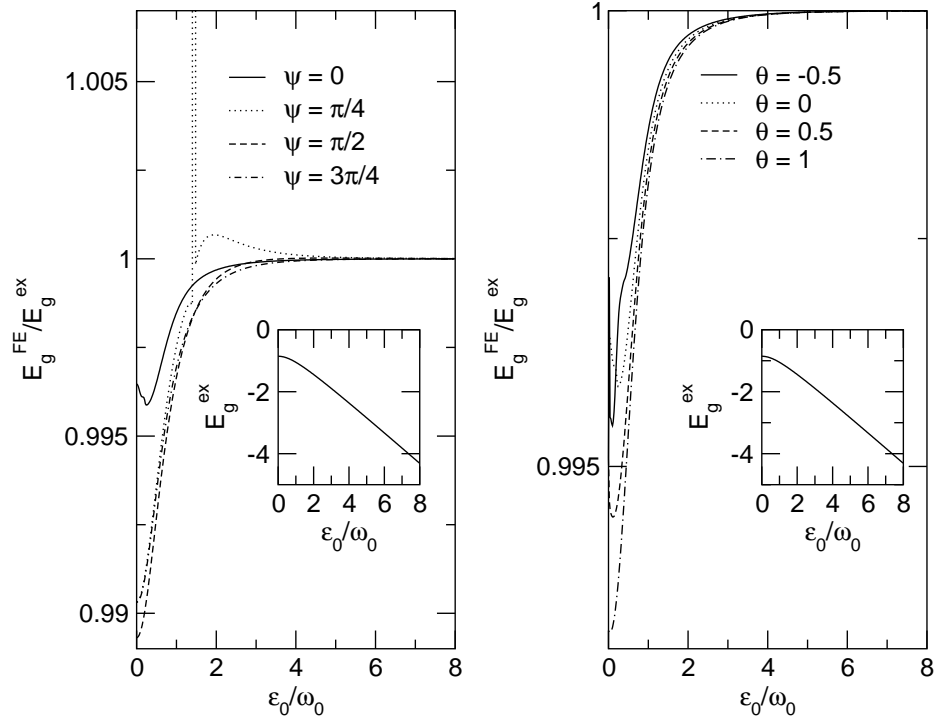
FIG. 3: The ground-state energy E_g^{FE} obtained by the canonical generator of Version b for $\Delta_0/\omega_0 = 1.5$ and $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel. The expectation values for the bosonic shift $\delta = \sum_j \langle \sigma_j \rangle \lambda^j / \omega_0$ were evaluated directly according to Eqs. (25). The initial values were $\theta = 0$ and various ψ (left hand side) and $\psi = 0$ and various θ (right hand side).

Again the parameters of the generator are only defined up to a common factor. Choosing $\eta^e = 0$, $\eta^x = -\omega_0 \lambda^x f/2$, $\eta^z = -\omega_0 \lambda^z f/2$ renders $\mathcal{O}_5$ zero and yields $\eta^{0,y} = \lambda^x \lambda^z f 1_n/2$ and $\eta^y = -R\lambda^x f/2$. Thus all neglected operators but $\mathcal{O}_1$ and $\mathcal{O}_2$ are zero. We obtain the following flow equations:

$$\partial_\ell R = -R\lambda^{x\,2} f 1_n \quad , \quad \partial_\ell E = -\omega_0(\lambda^{x\,2} + \lambda^{z\,2})f/2 \tag{31}$$
$$\partial_\ell \lambda^x = -\omega_0^2 \lambda^x f + R^2 \lambda^x f - \lambda^{z\,2} \lambda^x f 1_n \quad , \quad \partial_\ell \lambda^z = -\omega_0^2 \lambda^z f + \lambda^{x\,2} \lambda^z f 1_n$$

The set of equations in (31) is equivalent to the set of equations in (29). This can be seen by introducing "new" variables $\Delta' = \lambda^x R/\lambda'$, $\epsilon' = \lambda^z R/\lambda'$ and $\lambda'^2 = \lambda^{x\,2} + \lambda^{z\,2}$ and setting up their differential equations, which coincide with (29). This demonstrates that keeping the Hamiltonian form-invariant during the flow preserves the unitary equivalence with respect to the initial Hamiltonian for this special unitary transformation.

If we want the initial Hamiltonian to remain form-invariant during the flow after having shifted the bosonic mode by θ, the constants have to satisfy the following relations:

$$-\epsilon \eta^y + \eta^x \omega_0 - \eta^{0,y} \lambda^z + 2\eta^y \lambda^z \delta = 0 \tag{32}$$
$$-\Delta \eta^z - \epsilon \eta^x + \eta^y \omega_0 + 2\eta^x \lambda^z \delta = 0 \tag{33}$$

After the shift, λ^e is naturally generated which was not present in the previous schemes. In order to compare the flow equations with the above versions, we have to couple the flow of λ^e with the flow of λ^z, i.e. $\lambda^e = \theta \lambda^z$. This sets another condition on the parameters of the generator, i.e. $\eta^e = -\theta \Delta \eta^y / \omega_0 + \theta \eta^z$. If we further choose $\eta^y = -\Delta \lambda^z f/2$ we obtain $\eta^z = -\omega_0 \lambda^z f/2$, $\eta^x = 0$, $\eta^{0,y} = \epsilon \Delta f/2 - \Delta \lambda^z \delta f$ and $\eta^e = \theta \Delta^2 \lambda^z f/(2\omega_0) - \theta \omega_0 \lambda^z f/2$ with the factor f to be determined later. With $\bar{\epsilon} = \epsilon - \theta \lambda^{z\,2}/\omega_0$, this yields the following flow equations :

$$\partial_\ell \Delta = -\Delta \lambda^{z\,2} f 1_n + \Delta(\bar{\epsilon} + \lambda^z(\delta - \theta\lambda^z/\omega_0))^2 f \quad , \quad \partial_\ell \bar{\epsilon} = -\Delta^2 \bar{\epsilon} f + 2\Delta^2 \lambda^z(\delta - \theta\lambda^z/\omega_0)f \quad ,$$
$$\partial_\ell \lambda^z = \lambda^z(\Delta^2 - \omega_0^2)f \quad , \quad \partial_\ell E = -\omega_0 \lambda^{z\,2} f/2 + \theta^2(\Delta^2 - \omega_0^2)\lambda^{z\,2} f/(2\omega_0) \tag{34}$$

Recalling the initial condition of the energy shift $E_0' = E_0 + \theta^2 \lambda_0^2/(4\omega_0)$ defined in Eq. (7) we see that the flow equations are equivalent to the flow equations of Version d if we set $f = 1$ and $\delta = \lambda^e/\omega_0 = \theta\lambda^z/\omega_0$. This choice of the ℓ-dependent shift coincides with the expression (24) if we set $\langle \sigma_z \rangle = 0$.
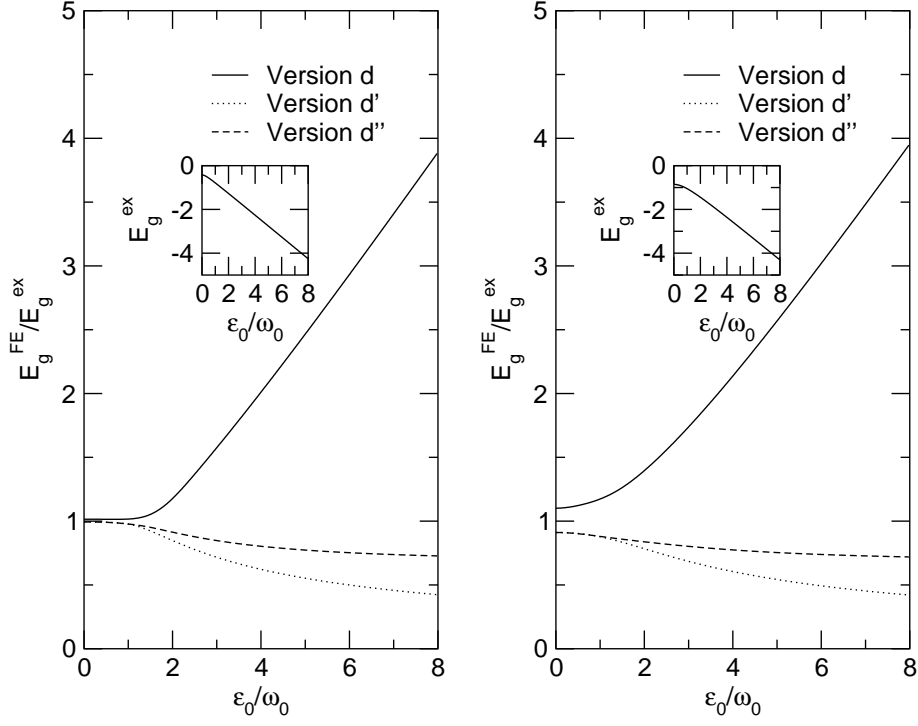
FIG. 4: The ground-state energy E_g^{FE} obtained from the form-invariant flow for $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact ground-state energy E_g^{ex}, shown in the panel. The primed versions are including the flow of the neglected operators $\mathcal{O}_1$ and $\mathcal{O}_2$ (see text).

This is a remarkable result. It shows that if one imposes invariance of the flow equations with respect to unitarily equivalent initial Hamiltonians and chooses the truncation scheme that leaves the Hamiltonian form-invariant, the flow equations are uniquely determined. It also shows that normal ordering with respect to the ℓ-dependent mode $\bar{b} = b + \delta$ leads to reasonable results.

We now want to check the quality of the form-invariant truncation scheme. In Figure 4 the ground-state energy E_g^{FE} obtained by the set of equations (29) is shown relative to the exact ground-state energy E_g^{ex} for two different tunnel-matrix elements $\Delta_0/\omega_0 = 0.5$ (left hand side) and $\Delta_0/\omega_0 = 1.5$ (right hand side). Drastic deviations from the exact result are seen in the regime $\epsilon_0/\omega_0 \geq 1$. This means that the neglected operator $\mathcal{O}_1$ of Eq. (16) becomes relevant and has to be taken into account.

In order to demonstrate that the flow equations can be improved systematically, we will now consider higher order terms of the bosonic operators in their normal ordered representation. For the normal ordering procedure see Appendix E. Since we set $\delta = 0$ for all ℓ, normal ordering is defined with the respect to the unshifted mode, i.e. $\bar{b} = b$. Redefining $\mathcal{O}_1 \equiv \sigma_x \kappa_1 : (b + b^\dagger)^2 :$, the commutator $[\eta, \mathcal{O}_1]$ yields

$$
\begin{aligned}
[\eta, \mathcal{O}_1] = {}& 2\sigma_z \eta^{y,0} \kappa_1 : (b + b^\dagger)^2 : + 2\sigma_z \eta^y \kappa_1 (: (b + b^\dagger)^3 : + 2\langle (b + b^\dagger)^2 \rangle : (b + b^\dagger) :) \\
& + 2i\sigma_y \eta^z \kappa_1 : (b - b^\dagger)(b + b^\dagger)^2 : \quad .
\end{aligned}
\tag{35}
$$

We first neglect the trilinear operators and the bilinear operator of type $\mathcal{O}_2$ (see Eq. (16)). The extended flow equations then read ($f = 1$)

$$
\begin{aligned}
&\partial_\ell \Delta = -\Delta \lambda^{z\,2} 1_n + \Delta \epsilon^2 \quad , \quad \partial_\ell \epsilon = -\epsilon \Delta^2 \quad , \quad \partial_\ell \kappa_1 = \Delta \lambda^{z\,2}/2 \\
&\partial_\ell \lambda^z = \lambda^z (\Delta^2 - \omega_0^2) + 4\lambda^z \Delta \kappa_1 1_n \quad , \quad \partial_\ell E = -\omega_0 \lambda^{z\,2} f/2 \quad .
\end{aligned}
\tag{36}
$$

We will refer to this set of flow equations as Version d$'$.

To see if this improvement is systematic we will now include also the corrections that come from the neglected operator of type $\mathcal{O}_2$. Redefining $\mathcal{O}_2 \equiv \sigma_z \kappa_2 : (b + b^\dagger)^2 :$, we obtain similar commutator relations for $[\eta, \mathcal{O}_2]$ as we got

in (35):

$$[\eta, \mathcal{O}_2] = -2\sigma_x \eta^{y,0} \kappa_2 : (b + b^\dagger)^2 : -2\sigma_x \eta^y \kappa_2 (: (b + b^\dagger)^3 : +2\langle (b + b^\dagger)^2 \rangle : (b + b^\dagger) :)$$
$$- 2i\sigma_y \eta^z \kappa_2 : (b - b^\dagger)(b + b^\dagger)^2 : \tag{37}$$

The effect of including the operator $\mathcal{O}_2$ in the flow equations is the following: The conditions for the constants of the generator that assure the form-invariance of the Hamiltonian slightly change, see Eq. (28). The flow equations thus read ($f = 1$)

$$\partial_\ell \Delta = -\Delta \lambda^{z2} 1_n + \Delta \epsilon (\epsilon + 4\kappa_2) \quad , \quad \partial_\ell \epsilon = -(\epsilon + 4\kappa_2) \Delta^2$$
$$\partial_\ell \lambda^z = \lambda^z (\Delta^2 - \omega_0^2) + 4\lambda^z \Delta \kappa_1 1_n \quad , \quad \partial_\ell E = -\omega_0 \lambda^{z2} f/2 \tag{38}$$
$$\partial_\ell \kappa_1 = \Delta \lambda^{z2}/2 - \Delta(\epsilon + 4\kappa_2)\kappa_2 \quad , \quad \partial_\ell \kappa_2 = \Delta(\epsilon + 4\kappa_2)\kappa_1 \quad .$$

We will refer to this set of flow equations as Version d''.

In Fig. 4 one sees that the extended flow equations yield a systematic improvement ranging over the whole parameter space. Nevertheless, the agreement with the exact result remains rather poor for $\epsilon_0/\omega_0 \geq 1$. Only if one considers the renormalization of the bath mode ω_0, one obtains results within a few percent relative error over the whole parameter range. Regarding the spin-boson model, it is preferable to employ the canonical generator since the bath modes remain unrenormalized in the thermodynamic limit[21].

III. FLOW OF OBSERVABLES

We will now investigate the flow of observables. In order to characterize the quality of the flow equations, normally sum rules are derived expressing the fact that $\sigma_i^2 = 1$ or (anti-)commutation relations should hold for all ℓ with $i = x, y, z$[5,7]. As will be pointed out in the end of this section, these sum rules can be misleading. We will therefore contrast the expectation value $\langle \sigma_z \rangle$ as it follows from the flow equation approach with the numerically exact solution. Furthermore, we will compare the flow equation results with the numerically exact fixed point of the operator flow on the operator level. To do so, we will give a unique decomposition of the fixed point operator into a basis of normal ordered bosonic operators.

A. Flow Equations for the Pauli Matrices

In order to take advantage of the simple form of the fixed point Hamiltonian when calculating expectation values of observables, the observable has to be subjected to the same sequence of unitary transformations as the Hamiltonian. The flow equations for the Pauli spin matrices thus read $\partial_\ell \sigma_i = [\eta, \sigma_i]$. Again the flow equations generate an infinite series of operators and one needs a suitable truncation and decoupling scheme. The i-component of the Pauli spin matrices as a function of the flow parameter ℓ shall be given by

$$\sigma_i(\ell) = g_i(\ell)\sigma_x + h_i(\ell)\sigma_z + f_i(\ell) + \sigma_x \chi^{x,i}(\ell)(b + b^\dagger) + i\sigma_y \chi^{y,i}(\ell)(b - b^\dagger) + \sigma_z \chi^{z,i}(\ell)(b + b^\dagger) \quad , \tag{39}$$

with $i = x, z$. We want to emphasizes that the constant term f_i is indeed generated even though it seems to contradict the theorem of the invariance of the trace under unitary transformations. A short discussion is given in Appendix B.

The flow of the y-component of the Pauli spin matrices is given by

$$i\sigma_y(\ell) = g_y(\ell)i\sigma_y + \sigma_x \chi^{x,y}(b - b^\dagger) + \sigma_z \chi^{z,y}(b - b^\dagger) \quad . \tag{40}$$

These are the most general expansions up to linear bosonic operators with real coefficients that can evolve from the Pauli spin matrices under the flow equations, i.e. from $\sigma_i(\ell = 0) = \sigma_i$.

The commutator $[\eta, \sigma_i]$ with $i = x, z$ yields the following contributions:

$$[\eta^{0,y}, \sigma_i(\ell)] = 2\sigma_z g_i \eta^{0,y} - 2\sigma_x h_i \eta^{0,y} + 2\sigma_z \eta^{0,y} \chi^{x,i}(b + b^\dagger) \tag{41}$$
$$- 2\sigma_x \eta^{0,y} \chi^{z,i}(b + b^\dagger)$$

$$[\eta^e, \sigma_i(\ell)] = 2\sigma_x \eta^e \chi^{x,i} + 2\sigma_z \eta^e \chi^{z,i} \tag{42}$$

$$[\eta^x, \sigma_i(\ell)] = -2i\sigma_y h_i \eta^x (b - b^\dagger) + 2\eta^x \chi^{x,i} - 2\sigma_z \eta^x \chi^{y,i}(b - b^\dagger)^2 \tag{43}$$
$$- i\sigma_y \eta^x \chi^{z,i}\{(b - b^\dagger),(b + b^\dagger)\}$$

$$[\eta^y, \sigma_i(\ell)] = 2\sigma_z g_i \eta^y (b + b^\dagger) - 2h_i \sigma_x \eta^y (b + b^\dagger) \tag{44}$$
$$+ 2\sigma_z \eta^y \chi^{x,i}(b + b^\dagger)^2 + 2\eta^y \chi^{y,i} - 2\sigma_x \eta^y \chi^{z,i}(b + b^\dagger)^2$$

$$[\eta^z, \sigma_i(\ell)] = 2i\sigma_y g_i \eta^z (b - b^\dagger) + i\sigma_y \eta^z \chi^{x,i}\{(b - b^\dagger),(b + b^\dagger)\} \tag{45}$$
$$+ 2\sigma_x \eta^z \chi^{y,i}(b - b^\dagger)^2 + 2\eta^z \chi^{z,i}$$

The commutator $[\eta, i\sigma_y]$ is given by:

$$[\eta^{0,y}, \sigma_y(\ell)] = 2\sigma_z \eta^{0,y} \chi^{x,y}(b - b^\dagger) - 2\sigma_x \eta^{0,y} \chi^{z,y}(b - b^\dagger) \tag{46}$$

$$[\eta^x, \sigma_y(\ell)] = -2\sigma_z g_y \eta^x (b - b^\dagger) - 2i\sigma_y \eta^x \chi^{z,y}(b - b^\dagger)^2 \tag{47}$$

$$[\eta^y, \sigma_y(\ell)] = \sigma_z \eta^y \chi^{x,y}\{(b + b^\dagger),(b - b^\dagger)\} - \sigma_x \eta^y \chi^{z,y}\{(b + b^\dagger),(b - b^\dagger)\} \tag{48}$$

$$[\eta^z, \sigma_y(\ell)] = 2\sigma_x g_y \eta^z (b - b^\dagger) + 2i\sigma_y \eta^z \chi^{x,y}(b - b^\dagger)^2 \tag{49}$$

Again, $\{.,.\}$ denotes the anti-commutator. To understand which operators can transform into one another, we give a list of operators and their behavior under parity transformation (P) and Hermitian conjugation (H) ($x \equiv (b + b^\dagger)$, $p \equiv (b - b^\dagger)$) :

	1	σ_x	$i\sigma_y$	σ_z	x	p	$\sigma_x x$	$\sigma_x p$	$i\sigma_y x$	$i\sigma_y p$	$\sigma_z x$	$\sigma_z p$
P	+	+	−	−	+	−	−	−	+	+	+	+
H	+	+	−	+	+	−	+	−	−	+	+	−

In order to close the flow equations, we neglect normal ordered bosonic bilinears where normal ordering is defined with respect to the shifted bosonic mode $\bar{b} = b + \delta/2$. Thus, one obtains the following set of linear differential equations for the i-component of the Pauli spin matrices with $i = x, z$:

$$\partial_\ell g_i = -2h_i \eta^{0,y} + 2\eta^e \chi^{x,i} - 2\eta^z \chi^{y,i} 1_n - 2\eta^y \chi^{z,i} 1_n + 2\eta^y \chi^{z,i} \delta^2 \tag{50}$$

$$\partial_\ell h_i = 2g_i \eta^{0,y} + 2\eta^y \chi^{x,i} 1_n + 2\eta^x \chi^{y,i} 1_n + 2\eta^e \chi^{z,i} - 2\eta^y \chi^{x,i} \delta^2 \tag{51}$$

$$\partial_\ell f_i = 2\eta^x \chi^{x,i} + 2\eta^y \chi^{y,i} + 2\eta^z \chi^{z,i} \tag{52}$$

$$\partial_\ell \chi^{x,i} = -2h_i \eta^y - 2\eta^{0,y} \chi^{z,i} + 4\eta^y \chi^{z,i} \delta \tag{53}$$

$$\partial_\ell \chi^{y,i} = 2g_i \eta^z - 2h_i \eta^x + 2\eta^x \chi^{z,i} \delta - 2\eta^z \chi^{x,i} \delta \tag{54}$$

$$\partial_\ell \chi^{z,i} = 2g_i \eta^y + 2\eta^{0,y} \chi^{x,i} - 4\eta^y \chi^{x,i} \delta \tag{55}$$

The flow equations for the y-component read:

$$\partial_\ell g_y = -2\eta^z \chi^{x,y} 1_n + 2\eta^x \chi^{z,y} 1_n \tag{56}$$

$$\partial_\ell \chi^{x,y} = 2g_y \eta^z - 2\eta^{0,y} \chi^{z,y} - 2\eta^y \chi^{z,y} \delta \quad , \quad \partial_\ell \chi^{z,y} = -2g_y \eta^{0,y} x + 2\eta^{0,y} \chi^{x,y} - 2\eta^y \chi^{x,y} \delta \tag{57}$$

If no approximation was made, $\sigma_i^2(\ell) = 1$ would hold for all ℓ and $i = x, y, z$. Taking the expectation value with respect to the bilinear Hamiltonian of the shifted modes the relation should hold approximately for $i = x, z$:

$$\langle \sigma_i^2(\ell) \rangle = g_i^2 + h_i^2 + f_i^2 + (\chi^{x,i}\chi^{x,i} + \chi^{y,i}\chi^{y,i} + \chi^{z,i}\chi^{z,i})1_n$$
$$+ 2(g_i \langle \sigma_x \rangle + h_i \langle \sigma_z \rangle)f_i + 2(\chi^{x,i}\langle \sigma_z \rangle - \chi^{z,i}\langle \sigma_x \rangle)\chi^{y,i}$$
$$+ (\chi^{x,i}\chi^{x,i} + \chi^{z,i}\chi^{z,i})\delta^2 - 2((g + \langle \sigma_x \rangle f)\chi^{x,i} + (h + \langle \sigma_z \rangle f)\chi^{z,i})\delta \tag{58}$$
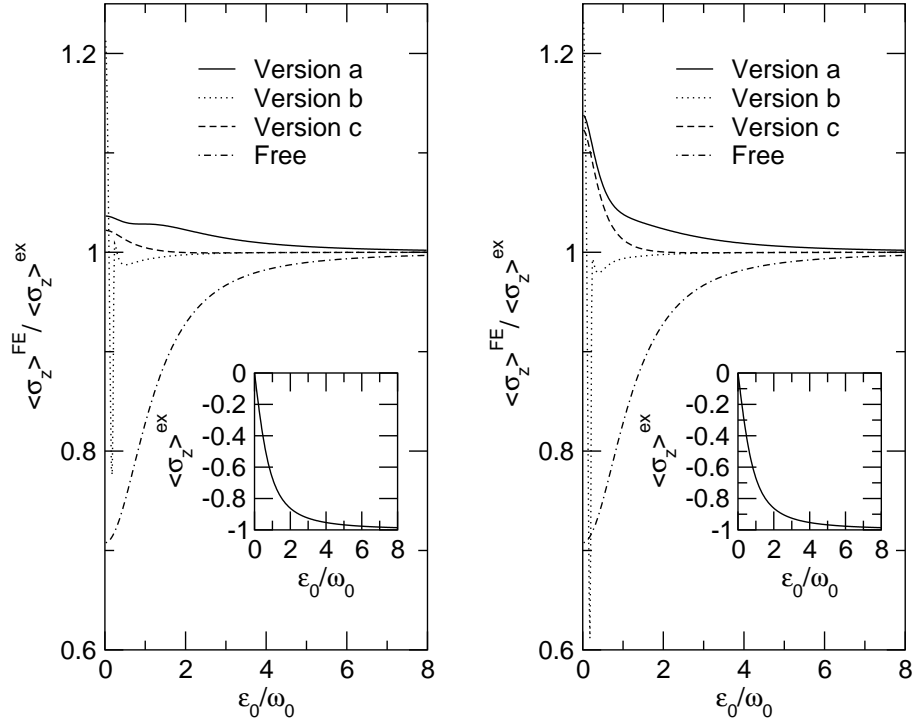$$\approx 1$$

FIG. 5: The expectation value $\langle \sigma_z \rangle^{FE}$ obtained by different canonical generators with $\psi = 0$ and $\theta = 0$ for $\Delta_0/\omega_0 = 1.5$ with $\lambda_0/\omega_0 = 1$ as function of the bias ϵ_0 relative to the exact expectation value $\langle \sigma_z \rangle^{ex}$, shown in the panel. The expectation values for the bosonic shift $\delta = \sum_j \langle \sigma_j \rangle \lambda^j / \omega_0$ were evaluated directly according to Eqs. (25) (left hand side) and self-consistently according to Eqs. (27) (left hand side).

For the y-component we obtain:

$$\langle \sigma_y^2(\ell) \rangle = g_y^2 + (\chi^{x,y}\chi^{x,y} + \chi^{z,y}\chi^{z,y})1_n \approx 1 \tag{59}$$

Other conservation relations follow e.g. from the commutator $[\sigma_x(\ell), \sigma_z(\ell)] = -2i\sigma_y(\ell)$. These relations can be used to assess the validity and the quality of the flow equations but they cannot assure whether the scheme will yield the correct results. We will comment on this point at the end of this section.

B.   Numerical Results for the Expectation Value of σ_z

Measurable quantities other than the ground-state energy are determined by means of the operator flow. In this subsection we will discuss the expectation value $\langle \sigma_z \rangle$ as it follows from the different versions of the flow equation approach. The expression is given by

$$\langle \sigma_z \rangle = {}^*\langle \sigma_z(\ell = \infty) \rangle^* = g(\ell = \infty)^* \langle \sigma_x \rangle^* + h(\ell = \infty)^* \langle \sigma_z \rangle^* + f(\ell = \infty) \quad . \tag{60}$$

Here, ${}^*\langle ... \rangle^*$ denotes the ground-state expectation value with respect to the fixed point Hamiltonian $H(\ell = \infty)$.

In Fig. 5 we contrast the results for the different generators which were discussed in the last section, $\langle \sigma_z \rangle^{FE}$, with the numerically exact solution $\langle \sigma_z \rangle^{ex}$. We choose $\psi = 0$ and $\theta = 0$ for the initial Hamiltonian and we will employ the flow equations obtained by the generalized normal ordering procedure, i.e. $\delta = \sum_j \langle \sigma_j \rangle \lambda^j / \omega_0$.

On the left hand side of Fig. 5, the expectation values in the expression of δ are determined directly according to Eqs. 25. On the right hand side of Fig. 5, the expectation values are evaluated self-consistently according to Eqs. 27. For $\epsilon_0/\omega_0 \geq 1$, the best results are obtained by the generator of Version b with the direct evaluation of the expectation values. But deviations from the exact solution in the region $\epsilon_0/\omega_0 \leq 1$ are significant. In the latter region the generator of Version c yields the best results. We recall that the ground-state energy was best approximated by the generator of Version b with the self-consistent evaluation of the expectation values entering the bosonic shift δ.
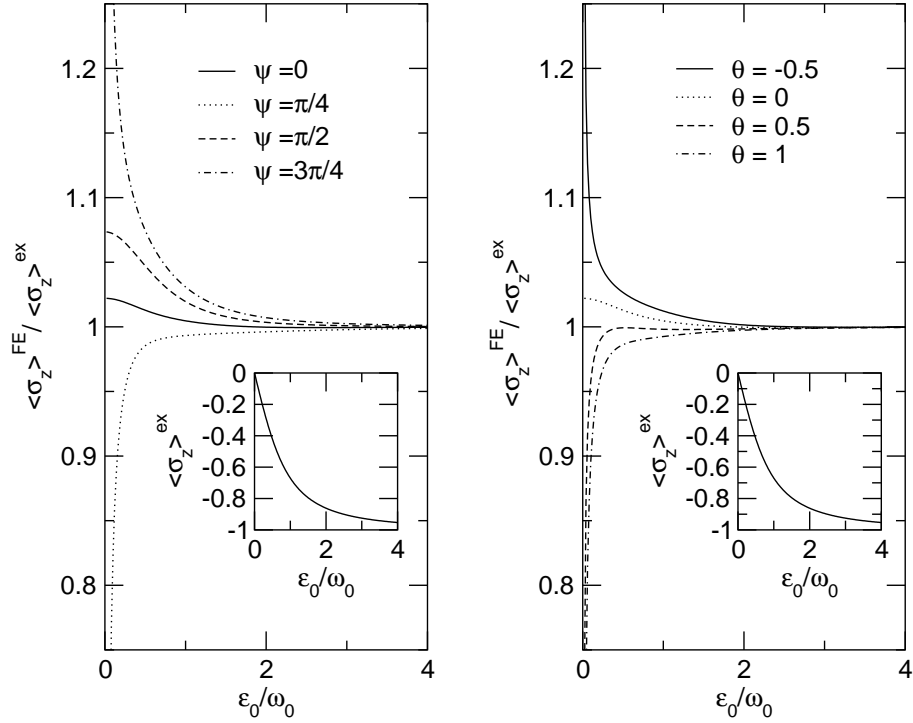
FIG. 6: The expectation value $\langle\sigma_z\rangle^{FE}$ obtained by the canonical generator of Version c with $\delta = \sum_j \langle\sigma_j\rangle\lambda^j/\omega_0$ for $\Delta_0/\omega_0 = 1.5$ and $\lambda_0/\omega_0 = 1$ as a function of the bias ϵ_0 relative to the exact expectation value $\langle\sigma_z\rangle^{ex}$, shown in the panel. The parameters of the initial Hamiltonian are given by $\theta = 0$ and various ψ (left hand side) and $\psi = 0$ and various θ (right hand side).

This demonstrates that the "best" generator and "best" procedures of taking account of the neglected terms might depend on the physical quantity under consideration.

We will now also include the initial unitary transformation on the two-dimensional spin-Hilbert space, label by ψ and the initial bosonic shift θ in our discussion. We will use the generator of Version c with the direct evaluation of the expectation values. On the left hand side of Fig. 6, we vary ψ with $\theta = 0$; on the right hand side of Fig. 6 we vary θ with $\psi = 0$.

Regardless the initial Hamiltonian, the flow equation results differ from the exact solution in the region $\epsilon_0/\omega_0 \leq 2$. But some initial Hamiltonians provoke more significant deviations than others. Good results over the whole parameter space are obtained by combining non-zero values of ψ and θ which "compensate" their errors, e.g. $\psi = \pi/32$ and $\theta = -0.2$. Nevertheless, we were not able to given an objective procedure how to choose the optimal initial Hamiltonian - a priori.

C.   Operator Fixed point

It is possible to compare the exact results with the flow equation approach not only on the spectral but also on the operator level. For this we have to diagonalize the Hamiltonian in this basis in which the corresponding "diagonal" Hamiltonian H_0 of the flow equation approach is diagonal. Let now $H_D = UHU^\dagger$ denote the diagonalized Hamiltonian, then $\sigma_i^* = U\sigma_i U^\dagger$ is the operator to be compared with $\sigma_i(\ell = \infty)$ stemming from the flow equation approach, with $i = x, y, z$. To do so we will decompose σ_i^* in a set of operators which are created by the corresponding flow equations.

If one uses an expansion which is normal ordered in the bosonic operators the decomposition can be obtained numerically without any approximation[22]. The reason for this is that the bosonic ladder operators cannot compensate each other and then act on lower bosonic subspaces. To make this more explicit the general matrix structure of a normal ordered operator consisting of N bosonic operators is shown on the left hand side of Figure 7, taking the set $\{|\nu\rangle\}$ as basis with $|\nu\rangle \equiv (b^\dagger)^\nu/\sqrt{\nu!}|0\rangle$ and $b|0\rangle = 0$, ν being a positive integer. The dark area contains non-zero entries whereas the white area contains no entries. In case of a non-normal ordered operator the white, upper left triangle would also contain non-zero entries.

As an explicit choice of the operator basis for real symmetric operators like σ_x and σ_z we choose the set $\{o :$
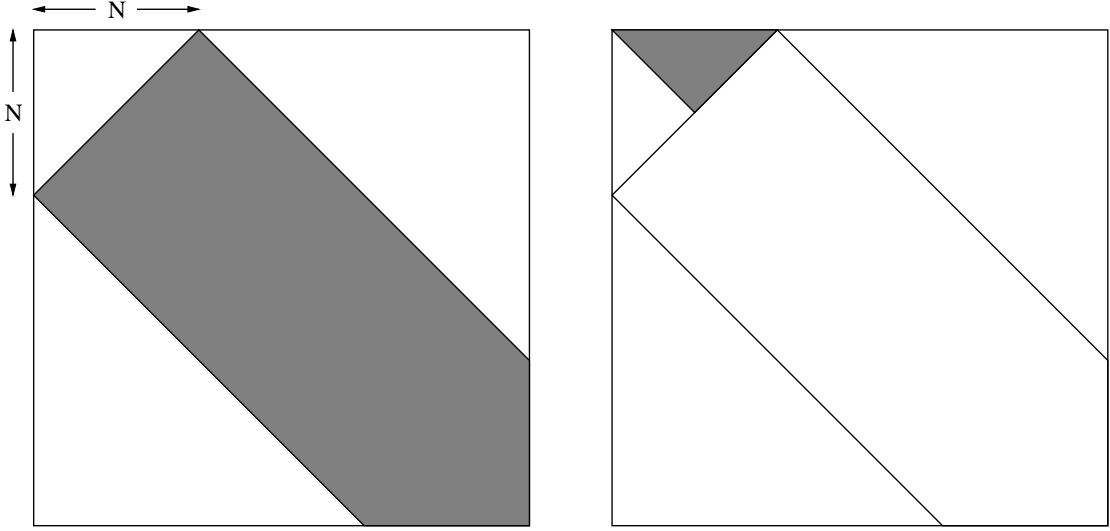
FIG. 7: Left hand side: Matrix structure of a normal ordered bosonic operator consisting of N bosonic operators with respect to the canonical basis (see text). The dark area indicates non-zero entries. Right hand side: The dark area indicates the matrix elements of an arbitrary matrix which are uniquely determined by normal ordered operators consisting of up to a certain number of bosonic operators (see text).

$(b + b^\dagger)^n (b - b^\dagger)^{2m} :, o' : (b + b^\dagger)^{n'} (b - b^\dagger)^{2m'+1} :\}$, where $o = 1, \sigma_x, \sigma_z$ and $o' = i\sigma_y$. The operator basis for real antisymmetric operators is obtained by interchanging o and o'. In the following we will only consider the flow of real symmetric operators. The results also hold for the real antisymmetric case.

We want to decompose a real symmetric operator into a set of finite operators. Considering all operators of the basis given above with less or equal than $2N$-bosonic operators, we obtain a finite basis of $3 \sum_{m=0}^{N} \sum_{n=0}^{2(N-m)} + \sum_{m'=0}^{N} \sum_{n'=1}^{2(N-m')} = (N+1)(4N+3)$ operators. Summing up the independent matrix elements which are uniquely determined by the normal ordered operators containing up to $2N$ bosonic modes, we obtain $\sum_{n=0}^{N} 2(4n+1) + 1 = 4(N+1)N + 3(N+1) = (N+1)(4N+3)$. These independent matrix elements are located at the upper left triangle of the matrix, indicated as dark area on the right hand side of Figure 7.

In order to complete the discussion we also consider all operators with less or equal than $(2N+1)$-bosonic operators. We then obtain a basis with $3 \sum_{m=0}^{N} \sum_{n=0}^{2(N-m)+1} + \sum_{m'=0}^{N} \sum_{n'=0}^{2(N-m')} = (N+1)(4N+7)$ operators. Summing up the independent matrix elements which are uniquely determined by the normal ordered operators containing up to $2N+1$ bosonic modes, we obtain $\sum_{n=0}^{N} 2(4n+3) + 1 = 4(N+1)N + 7(N+1) = (N+1)(4N+7)$.

We thus obtain the same number of independent matrix elements and basis "vectors". This confirms that our basis is complete and linearly independent as we take $N \to \infty$. Secondly, this shows that the first $(N+1)(4N+3)$ coordinates of a real symmetric operator with respect to a finite basis of operators up to $2N$ bosonic operators are left unchanged if one goes over to a finite basis including $2N + M$ bosonic operators ($M > 0$).

We can thus *exactly* determine the coefficients of our basis up to any number of bosonic excitations N which σ_i^* is composed of. This shows that choosing a set of normal ordered bosonic operators as a basis yields a systematic approximation of any operator. If one is only interested in the system dynamics at low energies it thus suffices to consider only up to N bosonic operators with $N = 2$ say.

To determine the coefficients numerically one has to work with a specific basis. Up to now we have only specified the basis of the bosonic Hilbert space. Choosing $H_0 = -\frac{\Delta_0}{2}\sigma_x + \omega_0 b^\dagger b$ to be diagonal we are led to the basis $\{|e, \nu\rangle\}$ with the first quantum number $e = 0, 1$ denoting the eigenstates of σ_x and the second quantum number denoting the eigenstates of $b^\dagger b$. Choosing $H_0 = \frac{\epsilon}{2}\sigma_z + \omega_0 b^\dagger b$ (Version 1b) or the diagonalized representation $H_0 = \frac{R}{2}\sigma_z + \omega_0 b^\dagger b$ of Version 1c, we would choose the first quantum number $e = 0, 1$ to denote the eigenstates of σ_z.

Considering all operators with less or equal than $2N$-bosonic operators, we end up to solve a linear equation $Ax = b$, with A being a quadratic matrix and x, b being vectors with dimensions $(N+1)(4N+3)$. The coefficients of the

matrix A are obtained by the following matrix representations of normal ordered bosonic operators:

$$\langle e, \mu | o : (b + b^\dagger)^n (b - b^\dagger)^{2m} : | e', \nu \rangle = \langle e | o | e' \rangle \sum_{k=0}^{n} \binom{n}{k} \sum_{l=0}^{2m} \binom{2m}{l} (-1)^{2m-l}$$

$$\times \, \Theta(\nu - k - l) \sqrt{\frac{\mu!}{(N-k-l)!}} \sqrt{\frac{\nu!}{(N-k-l)!}} \delta_{\mu, \nu + n + 2(m-k-l)} \tag{61}$$

The vector b on the right hand side of the linear equation is given by the $(N+1)(4N+3)$ independent matrix elements, located at the dark area of the matrix of the right hand side of Figure 7.

D. Higher Orders

In the expansion of the Pauli spin matrices of the last section we have neglected all generated operators with more than one bosonic operator. In order to confirm that the expansion of the Pauli spin matrices in normal ordered bosonic operators is indeed systematic we will now upgrade our expansion and also include:

- all generated operators up to two normal ordered bosonic operators

- all generated operators up to three normal ordered bosonic operators

In the following, normal ordering shall be defined with respect to the bilinear Hamiltonian of the un-shifted mode, i.e. $\delta = 0$. This will simplify matters considerably. Choosing the parameters of the initial Hamiltonian such that $\delta = 0$ for all ℓ, we are still consistent within our normal ordering procedure.

The first extension, $\sigma_z^{new,2}$, includes the following terms, where we introduce the abbreviations $x \equiv b + b^\dagger$ and $p \equiv b - b^\dagger$ and where we also confine ourself to the discussion of σ_z in order to drop one index:

$$\sigma_z^{new,2} = \chi^1 x + \sigma_x \psi^{x,+} : x^2 : + i\sigma_y \psi^{y,+} : xp :$$
$$+ \sigma_z \psi^{z,+} : x^2 : + \sigma_x \psi^{x,-} : p^2 : + \sigma_z \psi^{z,-} : p^2 : \tag{62}$$

The second extension, $\sigma_z^{new,3}$, consists of the following terms:

$$\sigma_z^{new,3} = \psi^{1,+} : x^2 : + \psi^{1,-} : p^2 : + \sigma_x \varphi^{x,+} : x^3 : + i\sigma_y \varphi^{y,+} : x^2 p :$$
$$+ \sigma_z \varphi^{z,+} : x^3 : + \sigma_x \varphi^{x,-} : xp^2 : + i\sigma_y \varphi^{y,-} : p^3 : + \sigma_z \psi^{z,-} : xp^2 : \tag{63}$$

The resulting flow equations for the upgraded truncation schemes are presented in Appendix C.

E. Numerical Results

We are now set to compare the fixed points of the operator flow obtained from the flow equation approach with the exact results. We can also see from the exact solution if the expansion into normal ordered bosonic operators is preferable.

It turns out that the expansion into normal ordered operators is not without obstacles. Especially when the reflection symmetry is broken, i.e. $\epsilon_0 \neq 0$, the final values of the coefficients delicately depend on the initial parameters of the Hamiltonian. The reason for this is that the unperturbed states cross when the interaction is switched on and this effects the representation of the operator. The effect is enhanced by explicitly breaking certain symmetries.

Also the comparison of the operator flow with respect to the different versions of the flow equations, discussed in the previous section, is troublesome. Since the non-trivial versions for $\epsilon = 0$ are based on different diagonal Hamiltonians H_0, a direct comparison of the fixed point parameters is not obvious.

We therefore limit our investigations to the parameter regime where the reflection symmetry is not broken, i.e. $\epsilon_0 = 0$. If we choose the generator of Version a with $\psi = 0$ and $\theta = 0$, $\delta = 0$ for all ℓ, and if we consider the flow of the z-component of the Pauli spin matrices, only two parameters h_z and $\chi^{x,z}$ are being renormalized. The final values $h_z^* \equiv h_z(\ell = \infty)$ and $\chi^{x,z*} \equiv \chi^{x,z}(\ell = \infty)$ are shown for the initial condition $\lambda_0/\omega_0 = 0.5$ in Figure 8, together with the results where we also included the flow of bilinear (2. order) and trilinear (3. order) bosonic operators, governed by Eqs. (C4) - (C13) and Eqs. (C14) - (C27).

The fixed point coefficients h_z^* and $\chi^{x,z*}$ agree with the exact solution unless the initial tunnel-matrix element Δ_0 is close to a resonance, i.e. $\Delta_0 \approx \omega_0$ or $\Delta_0 \approx 3\omega_0$[23]. The spike at $\Delta_0 \approx 3\omega_0$ cannot be accounted for by any of the
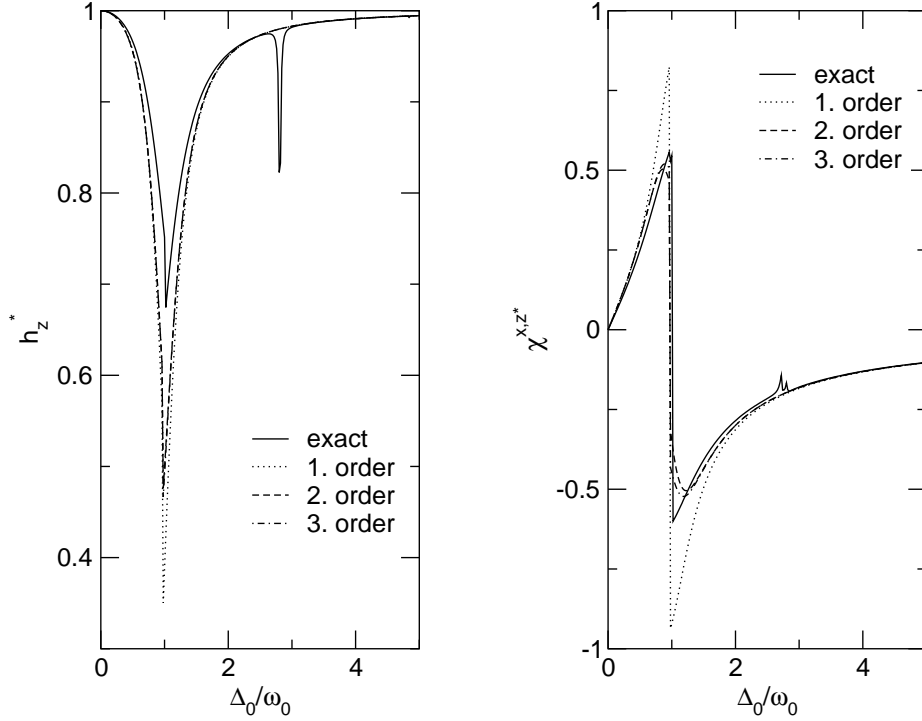
FIG. 8: The fixed point parameters $h_z^* \equiv h_z(\ell = \infty)$ (left hand side) and $\chi^{x,z*} \equiv \chi^{x,z}(\ell = \infty)$ stemming from the symmetric flow equations of Version a for $\psi = 0$, $\theta = 0$, $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ for different orders of truncation of the operator flow as a function of Δ_0. The solid lines resembles the exact result.

solutions obtained via flow equations. But there is a significant improvement from the second order to the first order result close to the resonance at $\Delta_0 \approx \omega_0$ especially in the case of $\chi^{x,z*}$. The improvement from third to second order in the case of $\chi^{x,z*}$ is not as strong and the one particle parameter h_z^* is almost left unchanged.

In Figure 9, the results for the fixed point operator σ_x^* are shown as they follow from the flow equations of Version a with the initial conditions $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$. Four parameters $g_x^* \equiv g_x(\ell = \infty)$, $f_x^* \equiv f_x(\ell = \infty)$, $\chi^{y,x*} \equiv \chi^{y,x}(\ell = \infty)$, and $\chi^{z,x*} \equiv \chi^{z,x}(\ell = \infty)$ are generated during the flow. They show the same deficiencies with respect to the exact solution as the results of Figure 8. We want to mention that the constant term f_x^* is indeed generated, as can be seen from the exact expansion.

To investigate the reason for the above discrepancies close to resonances further, we are going to employ the numerically exact solution and determine the expansion of the final operator $\sigma_z^* = U\sigma_z U^\dagger$ including up to nine bosonic operators. Instead of analyzing the graphs of all 115 coefficients, we will consider the sum of the absolute values of the coefficients that belong to the operator class which consists of n bosonic operators (nth-order).

The resulting nine graphs are shown in Figure 10. As can be seen, the second order still contributes to the fixed point operator considerably. Close to resonances even higher orders become important for the operator expansion. This explains why the fixed point parameter h_z^* is not sufficiently recovered by the flow equation approach even after including all terms up to three bosonic operators into the flow equations.

In Appendix D, the spikes of Figure 10 are related to degeneracies. The formalism thus breaks down at these parameter configurations. This is related to the problem that occurs when diagonalizing the Hamiltonian which is, strictly speaking, also only possible for non-degenerate states.

Let us finally comment on sum rules that stem from operator relations which remain invariant under unitary transformations. Taking the initial values for the Hamiltonian as in Figure 8, the flow equations of Version a yield the exact sum rule $\langle \sigma_z^2 \rangle = h^2 + (\chi^{x,z})^2 = 1$ at $T = 0$ for all ℓ and independent of the initial tunnel-matrix element Δ_0. The sum rule is thus not sensitive to the deviations between the flow equation results and the exact solution, which become especially drastic close to resonances, see Fig. 8. We observe the situation that two errors are being canceled to yield the desired result. We therefore conclude that the sum rule cannot be a sufficient criterion for the quality of the operator flow. On the other hand, one cannot expect that the flow equations yield good results on all energy scales. Properties at low energies like the ground-state expectation value of σ_z shown in Figs. 5 and 6 still can be calculated with high precision. The typical deviations at resonances in the operator flow are averaged out.
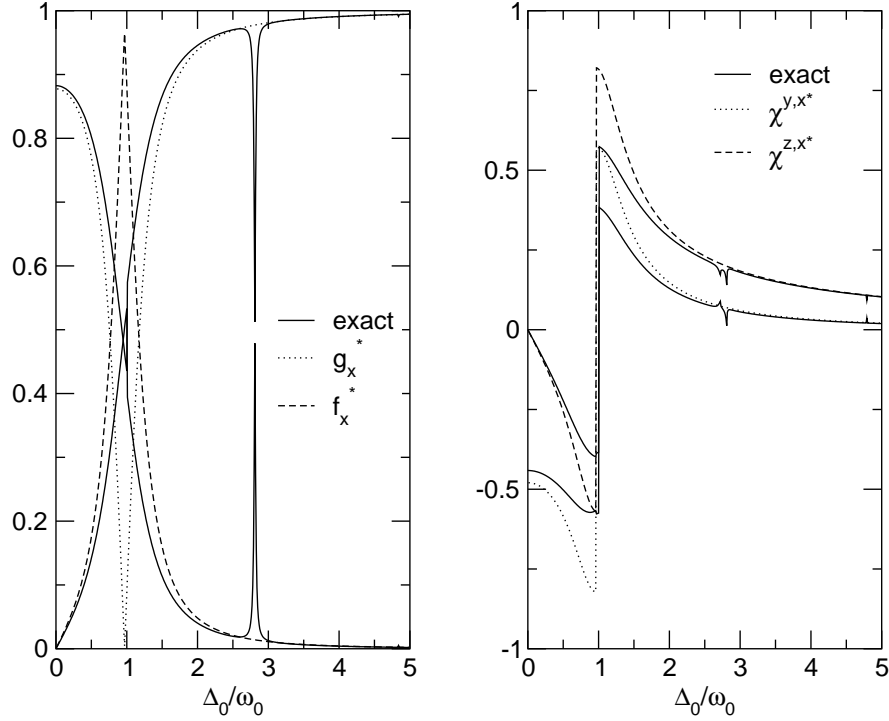
FIG. 9: The parameters $g_x^* \equiv g_x(\ell = \infty)$ and $f_x^* \equiv f_x(\ell = \infty)$ (left hand side) as well as $\chi^{y,x*} \equiv \chi^{y,x}(\ell = \infty)$ and $\chi^{z,x*} \equiv \chi^{z,x}(\ell = \infty)$ stemming from the symmetric flow equations of Version a for $\psi = 0$, $\theta = 0$, $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ as function of Δ_0. The solid lines resemble the analytic results.

IV. CONCLUSIONS

This work addresses general questions concerning the flow equation approach such as optimization of the final results or invariance with respect to the initial Hamiltonian, based on a simple non-trivial model. The model is structurally similar to quantum impurity models and since the "bath" only consists of one mode, it is numerically exactly solvable. We intended to demonstrate that a systematic improvement of the flow equation approach is possible. In order to improve the flow equations one can basically precede according to the following lines:

1. Most obviously, one can include more interaction terms in the truncation scheme of Hamiltonian and operator. This was done for the Hamiltonian flow when employing the form-invariant truncation scheme and a systematic improvement was seen. We did not extend the truncation scheme for the canonical generator because it is in principle not feasible for more realistic models with an arbitrary number of bosonic modes. For the operator flow, the truncation scheme was extended up to third order for a special parameter regime and the results were compared with the exact solution on the operator level. Close to resonances, the flow equation results showed significant deviations with respect to the exact solution . These deviations were present even in the upgraded truncation schemes since high orders of up to nine bosonic operators still carried considerable weight. This is connected to the general problem that the flow equation approach breaks down close to degenerate states.

2. Another way to improve the flow equations is to consider the neglected operators more thoroughly, i.e. to introduce a refined decoupling scheme. This was done by introducing a ℓ-dependent bosonic shift δ and neglecting normal ordered bilinear bosonic operators with respect to this shifted mode. The bosonic shift was deduced by formally diagonalizing the truncated Hamiltonian and than decoupling the "system" from the "bath". The decoupling process was not unambiguous and two different approaches were investigated. These were labeled as direct and self-consistent evaluation of the system expectation values. The self-consistent approach turned out to yield better results on the level of the Hamiltonian flow, the direct approach was preferable on the level of the operator flow.

3. A third possibility to obtain better results is to choose a different basis which the flow is defined on. As an example we want to mention the vertex flow introduced by Kehrein[24]. We investigated the operator flow with
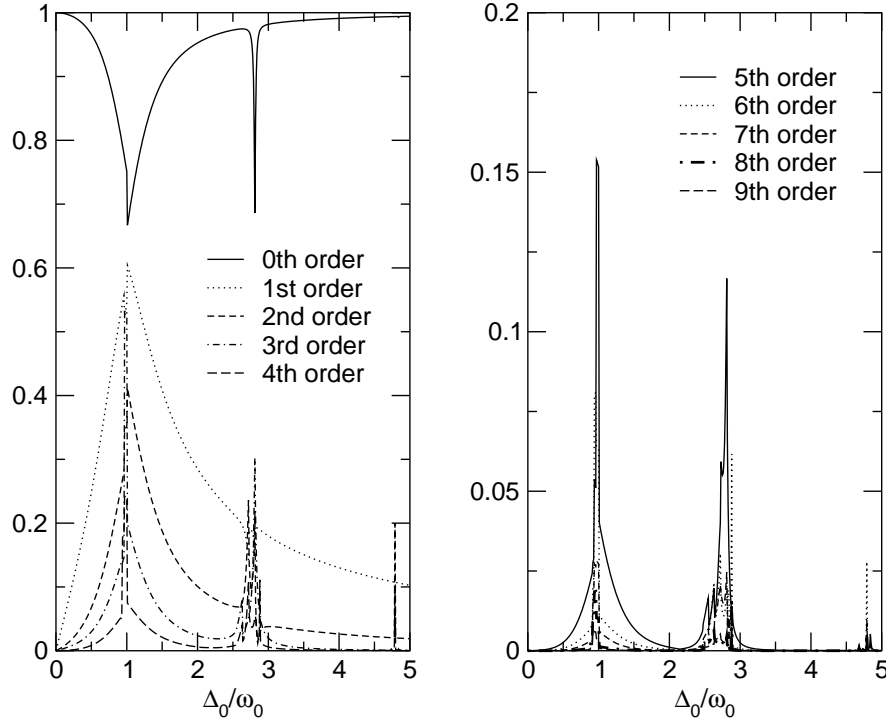
FIG. 10: The sum of the absolute values of the coefficients of all operators that consist of n bosonic operators (nth order) which compose σ_z^* for $\lambda_0/\omega_0 = 0.5$ and $\epsilon_0 = 0$ as function of Δ_0.

respect to the distinguished bosonic mode $\bar{b} = b + \delta/2$. The infinitesimal unitary transformations are then equivalent to an active *and* passive transformation since the coefficients as well as the operator basis $\bar{b}$ are changing during the flow. But the numerical results turned out to be worse than the ones based on the flow with respect to the unshifted mode b. We therefore did not include them in the discussion of the present paper. We want to emphasis, though, that there remains the possibility to improve the flow equation results along these lines.

It is also pointed out that flow equations are, in general, not invariant with respect to the initial Hamiltonian even though the Hamiltonians only differ by a unitary transformation. We concluded that differences are, in general, small and if one chooses a form-invariant truncation scheme, the flow equations might not differ at all. But the fact that the results depend on the unitary representation of the initial Hamiltonian opens up the possibility to optimize the results by introducing an (arbitrary) number of parameters associated with possible unitary transformations and choosing them such that certain sum rules are fulfilled best. This strategy has been applied to the spin-boson model with external bias, where one parameter - associated with the shift of the bosonic operators - was chosen such that the sum rule of σ_z was optimal for all ℓ.[21] What had to be left open was how to choose the optimal initial Hamiltonian for the evaluation of a specific quantity - *a priori*.

The last part of the paper is dedicated to a detailed analysis of the operator flow. Since the flow equations are usually designed such that the Hamiltonian is diagonalized best, i.e. that the flow only involves few flow parameters, the transformation of the observable is more susceptible to uncontrolled approximations, i.e. higher order interaction terms are often neglected merely because they cannot be kept track of. For this reason, the exact operator fixed point was evaluated, represented in the basis which was determined by the specific choice of the generator. It turned out that the flow equations of the operator should include up to 115 interaction terms in order to adequately coincide with the exact operator fixed point on all energy scales. We also pointed out that exact sum rules resulting from the flow equations are mostly due to high symmetries of the operator flow, i.e. when only few terms are being generated. The assumption that the flow is well approximated if a sum rule holds can thus be misleading as was shown in the last section. Nevertheless, the deviations at points of degeneracies of the operator flow with respect to the exact solution are unimportant for the low energy properties of the system. This was demonstrated by evaluating the ground-state expectation value of σ_z within the most simple, but non-trivial truncation scheme.

APPENDIX A: THE INDEPENDENT BOSON MODEL

We want to give a brief introduction to the flow equation method based on the exactly solvable Independent Boson Model. The Hamiltonian of this model is given by

$$H = H_0 + V = \omega b^\dagger b + \epsilon c^\dagger c + \lambda c^\dagger c(b + b^\dagger) \quad . \tag{A1}$$

The $b^{(\dagger)}$ resemble bosonic, the $c^{(\dagger)}$ fermionic operators. They obey the canonical commutation and anti-commutation relations respectively. The model can account for some relaxation phenomena and is extensively discussed in the textbook by Mahan[25].

We set $\epsilon = \lambda^2/\omega$. Then the Hamiltonian of Eq. (A1) is unitarily equivalent to $H = \omega b^\dagger b + \sigma_z \lambda(b + b^\dagger)$, where σ_z denotes the z-component of the Pauli spin matrices. This is the Rabi Hamiltonian (1) with $\Delta_0 = 0$.

The model is easily solved by the unitary transformation

$$U = \exp(-c^\dagger c \frac{\lambda}{\omega}(b - b^\dagger)) \tag{A2}$$

and we obtain the diagonalized Hamiltonian $UHU^\dagger = \omega b^\dagger b$.

But we want to perform this unitary transformation continuously by introducing a flow parameter ℓ and a family of unitarily equivalent Hamiltonians $H(\ell) = U(\ell)HU^\dagger(\ell)$. We also want to look closely at the transformed operator $c(\ell) \equiv U(\ell)cU^\dagger(\ell)$ and question if an expansion of the operator in a series of unbounded operators, namely $(b - b^\dagger)^n$, is well-defined.

The unitary operators $U(\ell)$ shall be defined by the generator η which governs the differential form of a continuous unitary transformations as follows: $\partial_\ell H = [\eta, H]$. A good choice for the generator has proven to be $\eta = [H_0, V]$, which is likely to eliminate the interaction in the limit $\ell \to \infty$[2]. The ℓ-dependent unitary operator $U(\ell)$ is related to the generator η through the differential equation $\partial_\ell U = \eta U$ which can be formally integrated to yield $U(\ell) = \mathcal{L} \exp(\int_0^\ell d\ell' \eta(\ell'))$. The operator $\mathcal{L}$ denotes the ℓ-ordering operator, defined in the same way as the more familiar time-ordering operator T. In fact, the differential form of the flow equations has got the same structure as the Heisenberg equation of motion, but complete formal equivalence is only achieved for explicitly time-dependent Hamiltonians, since the generator η is explicitly ℓ-dependent.

For the independent boson model the canonical generator reads $\eta = -\omega\lambda c^\dagger c(b - b^\dagger)$ and we readily obtain

$$[\eta, H] = -\omega^2 \lambda c^\dagger c(b + b^\dagger) - 2\omega\lambda^2 c^\dagger c \quad . \tag{A3}$$

The following flow equations

$$\partial_\ell \lambda = -\omega^2 \lambda \quad , \quad \partial_\ell \epsilon = -2\omega\lambda^2 \tag{A4}$$

are integrated to yield $\lambda(\ell) = \lambda \exp(-\omega^2\ell)$ and $\epsilon(\ell) = \frac{\lambda^2}{\omega}\exp(-2\omega^2\ell)$. Since $[\eta(\ell), \eta(\ell')] = 0$, the ℓ-ordering operator L becomes trivial and we obtain for the ℓ-dependent unitary operator

$$U(\ell) = \exp(-c^\dagger c \frac{\lambda}{\omega}(1 - e^{-\omega^2\ell})(b - b^\dagger)) \quad . \tag{A5}$$

From Eq. (A5) we can obtain the unique unitary operator for $\ell \to \infty$ which diagonalizes H and which was already given in Eq. (A2).

Given $U(\ell)$ one can determine the flow of the operator $c(\ell)$ directly:

$$c(\ell) = U(\ell)cU^\dagger(\ell) = c \exp(\frac{\delta\lambda(\ell)}{\omega}(b - b^\dagger)) \tag{A6}$$

$$= c \exp(-\frac{1}{2}\left(\frac{\delta\lambda(\ell)}{\omega}\right)^2) \exp(-\frac{\delta\lambda(\ell)}{\omega}b^\dagger) \exp(\frac{\delta\lambda(\ell)}{\omega}b) \tag{A7}$$

$$\equiv c \exp(-\frac{1}{2}\left(\frac{\delta\lambda(\ell)}{\omega}\right)^2) \sum_{n=0} \left(\frac{\delta\lambda(\ell)}{\omega}\right)^n \frac{: (b - b^\dagger)^n :}{n!} \quad , \tag{A8}$$

where we introduced $\delta\lambda(\ell) = \lambda(1 - e^{-\omega^2\ell})$ and defined normal ordering, denoted by : ... :, by writing the creation operator left from the annihilation operator. This definition of normal ordering resembles a special case of the general definition given in Appendix A and is valid at $T = 0$. But from now on the general definition will be used.

We now apply the continuous transformation to the operator c using the differential form $\partial_\ell c = [\eta, c]$. The flow equations generate the infinite series $c(\ell) = c\sum_{n=0}\gamma_n(\ell)(b - b^\dagger)^n$ with $\partial_\ell\gamma_{n+1} = \omega\lambda(\ell)\gamma_n$. Together with the initial condition $\gamma_0 = 1$, $\gamma_n = 0$ for $n \geq 1$, this set of differential equations can be solved to yield $\gamma_n = \frac{1}{n!}(\frac{\delta\lambda(\ell)}{\omega})^n$. The flow equation result thus coincides with the non-normal ordered form of $c(\ell)$ in Eq. (A6) if one expands the exponential function into a Taylor-series.

At first sight there is no distinguished expansion of $c(\ell)$ in bosonic operators since its generation depends on η. In order to discuss a different scheme, we now define $c(\ell)$ by a series of normal ordered operators, i.e. $c(\ell) = c\sum_{n=0}\gamma_n(\ell): (b - b^\dagger)^n :$. We obtain the following flow equations

$$\partial_\ell\gamma_{n+1} = \omega\lambda(\ell)(\gamma_n - (n+2)\gamma_{n+2}) \quad , \tag{A9}$$

where we used the formula (see Appendix E)

$$(b - b^\dagger) : (b - b^\dagger)^n :=: (b - b^\dagger)^{n+1} : +n\langle(b - b^\dagger)^2\rangle : (b - b^\dagger)^{n-1} : \tag{A10}$$

at $T = 0$, i.e. $\langle(b - b^\dagger)^2\rangle = -1$ with $\langle...\rangle$ denoting the bosonic ground-state expectation value. Taking the same initial conditions as in the case of the non-normal ordered expansion, we see that the normal ordered expansion in Eq. (A8) solves the set of differential equations (A9), i.e. $\gamma_n = \exp(-\frac{1}{2}(\delta\lambda(\ell)/\omega)^2)\frac{1}{n!}(\frac{\delta\lambda(\ell)}{\omega})^n$.

This is a remarkable result. Whereas the non-normal ordered expansion of $c(\ell)$ reproduces the perturbative result in the coupling $\delta\lambda$ for each coefficient γ_n, the normal ordered expansion yields coefficients γ_n, which contain all powers of $\delta\lambda$. Especially in view of later approximations, the normal ordered version will then be more preferable, since it is likely to go beyond a perturbative description.

After having recovered the correct flow of the observable via the flow equation approach, we would like to investigate the "stability" of the infinite expansion of $c(\ell)$ in unbounded operators. For this purpose, we consider the Green function $G(t) = -i\langle Tc(t)c^\dagger\rangle$ and the spectral function $A(\tilde\omega) = -\text{Im}G(\tilde\omega)/\pi$ with the time ordering operator T, the Fourier transform $G(\tilde\omega) = \int dt e^{i\tilde\omega t}G(t)$ and $\langle\ldots\rangle$ denoting the ground-state expectation value with respect to H. With $\tilde\lambda \equiv \lambda/\omega$ we obtain[25]

$$G(t) = -i\Theta(t)\exp(-\tilde\lambda^2(1 - e^{-i\omega t})) \quad , \tag{A11}$$

$$A(\tilde\omega) = e^{-\tilde\lambda^2}\sum_{n=0}\tilde\lambda^{2n}\frac{1}{n!}\delta(\tilde\omega - n\omega) \quad . \tag{A12}$$

The spectral function $A(\tilde\omega)$ thus exhibits the polaronic shift $\epsilon_p = -\lambda^2/\omega$ for $n = 0$ and an equidistant satellite structure separated by the oscillator frequency ω with exponentially decreasing weight.

Using flow equations, the Green function is best expressed as

$$G(t) = -i\Theta(t)\langle e^{iH(\ell=\infty)t}c^\dagger(\ell=\infty)e^{-iH(\ell=\infty)t}c(\ell=\infty)\rangle \quad , \tag{A13}$$

because then the time evolution of the fermionic and bosonic operator is that of free ones.

In order to recover the exact result, we first use the normal ordered expansion of $c(\ell)$. With $D(t) \equiv b(t) - b^\dagger(t)$, where the time evolution is given by the Heisenberg representation with $H(\ell = \infty) = \omega b^\dagger b$, the Green function reads:

$$G(t) = -i\Theta(t)e^{-\tilde\lambda^2}\langle c(t)\sum_{n=0}\frac{\tilde\lambda^n}{n!} : D^n(t) : c^\dagger\sum_{m=0}\frac{\tilde\lambda^m}{m!}(-1)^m : D^m(0) :\rangle \tag{A14}$$

$$= -i\Theta(t)e^{-\tilde\lambda^2}\sum_{n,m=0}\frac{\tilde\lambda^n}{n!}\frac{\tilde\lambda^m}{m!}(-1)^m\langle : D^n(t) :: D^m(0) :\rangle \tag{A15}$$

$$= -i\Theta(t)e^{-\tilde\lambda^2}\sum_{n,m=0}\frac{\tilde\lambda^n}{n!}\frac{\tilde\lambda^m}{m!}n!\delta_{n,m}e^{-in\omega t} \tag{A16}$$

To get from Eq. (A15) to Eq. (A16) we used the following formula (Appendix E):

$$: (b - b^\dagger)^n :: (b - b^\dagger)^m :=: \exp(\langle(b - b^\dagger)^2\rangle\frac{\partial^2}{\partial x_1\partial x_2})x_1^n x_2^m|_{x_1=x_2=(b-b^\dagger)} : \quad , \tag{A17}$$

with $\langle (b - b^\dagger)^2 \rangle = -1$ and $\langle : (b - b^\dagger)^n : \rangle = 0$ at $T = 0$. Summing up the series in Eq. (A16) indeed yields the exact result given in Eq. (A11).

In order to show that also the non-normal ordered expansion of $c(\ell)$ leads to the correct result, we have to normal order this expansion. For this we need the following formula (Appendix E):

$$(b - b^\dagger)^n = \sum_{k=0}^{[\frac{n-1}{2}]} \frac{1}{k!} \frac{n!}{2^k (n - 2k)!} \langle (b - b^\dagger)^2 \rangle^k : (b - b^\dagger)^{n-2k} : \qquad (A18)$$

Considering for the moment only the first $(N + 1)$ even powers of $(b - b^\dagger)$, we obtain

$$\sum_{n=0}^{N} \frac{\tilde{\lambda}^{2n}}{2n!} (b - b^\dagger)^{2n} = \sum_{n=0}^{N} \sum_{k=0}^{n} \frac{\tilde{\lambda}^{2k}}{2^k} \frac{G^k}{k!} \frac{\tilde{\lambda}^{2(n-k)}}{2(n-k)!} : (b - b^\dagger)^{2(n-k)} : \qquad (A19)$$

$$= \sum_{m=0}^{N} \frac{\tilde{\lambda}^{2m}}{2m!} : (b - b^\dagger)^{2m} : \sum_{k=0}^{N-m} \frac{\tilde{\lambda}^{2k}}{2^k} \frac{G^k}{k!} \qquad , \qquad (A20)$$

where we introduced $G \equiv \langle (b - b^\dagger)^2 \rangle$, $\langle ... \rangle$ denoting the canonical ensemble average over a free bosonic system . The summation of the first $(N + 1)$ odd powers of $(b - b^\dagger)$ yields

$$\sum_{n=0}^{N} \frac{\tilde{\lambda}^{2n+1}}{(2n+1)!} (b - b^\dagger)^{2n+1} = \sum_{m=0}^{N} \frac{\tilde{\lambda}^{2m+1}}{(2m+1)!} : (b - b^\dagger)^{2m+1} : \sum_{k=0}^{N-m} \frac{\tilde{\lambda}^{2k}}{2^k} \frac{G^k}{k!} \qquad . \qquad (A21)$$

In the limit $N \to \infty$ we obtain

$$\sum_{n=0}^{\infty} \frac{\tilde{\lambda}^n}{n!} (b - b^\dagger)^n = e^{\frac{1}{2} G \tilde{\lambda}^2} \sum_{n=0}^{\infty} \frac{\tilde{\lambda}^n}{n!} : (b - b^\dagger)^n : \qquad , \qquad (A22)$$

which is an extension of the previous normal ordering of Eq. (A8) to finite temperatures, since $G = -(1 + n)$, $n \equiv (e^{\beta \omega} - 1)^{-1}$ being the Bose factor. This shows that both expansions of $c(\ell)$ are equivalent.

To complete the discussion we will now verify that the anti-commutation relation $\{c(\ell), c^\dagger(\ell)\} = 1$ holds for all ℓ. To show this we will employ the non-normal ordered expansion. This yields

$$\{c(\ell), c^\dagger(\ell)\} = \frac{1}{2} \sum_{n,n'=0}^{\infty} \gamma_n \gamma_{n'} ((-1)^n + (-1)^{n'})(b - b^\dagger)^{n+n'} \qquad (A23)$$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{2n} (-1)^k \gamma_{2n-k} \gamma_k (b - b^\dagger)^{2n} = 1 \qquad . \qquad (A24)$$

Summarizing, the series expansion of an operator into bosonic operators yields consistent results. This is no trivial result since expanding the bounded operator c into unbounded operators $(b - b^\dagger)^n$ might have led to inconsistencies. Further, it has to be born in mind that the initial operator of the operator flow is resembled by $c(\ell = 0) = c \otimes 1_B$, with 1_B being the unity operator of the bosonic Hilbert space. One consequence then is that the trace of the initial operator is unbounded and thus not defined.

As a second result, we want to mention that both expansions, normal ordered and non-normal ordered, are equivalent if no approximations are involved. Nevertheless, the operator expansion into *normal ordered* operators seems to be a distinguished expansion since it resembles a non-perturbative approach including the Debye-Waller factor.

APPENDIX B: THE CONSTANT TERM IN THE EXPANSION OF σ_x AND σ_z

In this appendix we want to comment on the constant term f_i appearing in the expansion of the Pauli spin matrices σ_x and σ_z. This term seems to contradict the theorem of the invariance of the trace under unitary transformations. But since the trace of $\sigma_i(\ell = 0) = \sigma_i \otimes 1$, 1 being the identity of the bosonic Hilbert space, does not exist and since we also expand the Pauli spin matrices in a series of unbounded operators the above mentioned theorem does not hold anymore. To make sure that the constant term is indeed physical, one can truncate the Hilbert space by introducing the "bosonic" operator

$$b \to b_N = b \sqrt{(1 - b^\dagger b / N)} \qquad , \qquad (B1)$$

with N being a positive integer. The truncated Hilbert space is now only spanned by N vectors $|\nu\rangle = (b^\dagger)^\nu/\sqrt{\nu!}|0\rangle$ with $\nu = 0...N-1$ and $b|0\rangle = 0$. For $N \to \infty$ we recover the bosonic Hilbert space. The above theorem is guaranteed due to the new, non-canonical commutation relation $[b_N, b_N^\dagger] = 1 - (1 + 2b^\dagger b)/N$ which obeys the cyclic invariance of the trace:

$$\text{tr}([b_N, b_N^\dagger]) = \sum_{\nu=0}^{N-1} (1 - \frac{1+2\nu}{N}) = 0 \tag{B2}$$

The flow equations now have to be extended to include the flow of the operator $b^\dagger b$ that appears in the commutator relation and that scales as $1/N$. The constant term f_i appears nevertheless and is governed by the same differential equation as $N \to \infty$. Both terms together, the constant term f_i and the bosonic bilinear $b^\dagger b$, make sure that no trace is generated during the flow.

APPENDIX C: UPGRADED FLOW EQUATIONS FOR σ_z

In this Appendix, we will set up the flow equations for the Pauli matrix σ_z including higher orders in the bosonic operators. Since the basic objects of our expansion are normal ordered operators we will first give some (anti-)commutation relations which are helpful to evaluate the commutator $[\eta, \sigma_z]$ (see also Appendix E):

$$[x, : p^n x^m :] = -2n : p^{n-1} x^m : \quad , \quad [p, : p^n x^m :] = 2m : p^n x^{m-1} : \tag{C1}$$

$$\{x, : p^n x^m :\} = 2 : p^n x^{m+1} : +2m : p^n x^{m-1} : 1_n \tag{C2}$$

$$\{p, : p^n x^m :\} = 2 : p^{n+1} x^m : -2n : p^{n-1} x^m : 1_n \tag{C3}$$

The commutator of two tensor products of the fermionic and bosonic Hilbert space can be written as $[oB, o'B'] = \{o, o'\}[B, B']/2 + [o, o']\{B, B'\}/2$ which is a useful identity if the anti-commutator $\{o, o'\}$ vanishes ($o, o' \in \mathcal{H}_e$, $B, B' \in \mathcal{H}_b$).

We will not present the commutator $[\eta, \sigma_z]$ explicitly but only account for the additional terms that appear with respect to the previous flow equations. For the first extension $\sigma_z^{new,2}$, this yields:

$$\partial_\ell g_z = ... + 2\eta^x \chi^1 \quad , \quad \partial_\ell h_z = ... + 2\eta^z \chi^1 \tag{C4}$$

$$\partial_\ell \chi^x = ... - 2\eta^z \psi^y 1_n - 4\eta^y \psi^{z,+} 1_n \tag{C5}$$

$$\partial_\ell \chi^y = ... - 4\eta^z \psi^{x,-} 1_n + 4\eta^x \psi^{z,-} 1_n \tag{C6}$$

$$\partial_\ell \chi^z = ... + 2\eta^x \psi^y 1_n + 4\eta^y \psi^{x,+} 1_n \tag{C7}$$

$$\partial_\ell \chi^1 = 4\eta^z \psi^{z,+} - 2\eta^y \psi^y + 4\eta^x \psi^{x,+} \tag{C8}$$

$$\partial_\ell \psi^{x,+} = -2\eta^y \chi^z - 2\eta^{0,y} \psi^{z,+} \tag{C9}$$

$$\partial_\ell \psi^y = 2\eta^z \chi^x - 2\eta^x \chi^z \tag{C10}$$

$$\partial_\ell \psi^{z,+} = 2\eta^y \chi^x + 2\eta^{0,y} \psi^{x,+} \tag{C11}$$

$$\partial_\ell \psi^{x,-} = 2\eta^z \chi^y - 2\eta^{0,y} \psi^{z,-} \tag{C12}$$

$$\partial_\ell \psi^{z,-} = -2\eta^x \chi^y + 2\eta^{0,y} \psi^{x,-} \tag{C13}$$

Additional contributions relative to the previous flow equations coming from $\sigma_z^{new,3}$ read:

$$\partial_\ell \chi^x = ... + 4\eta^x \psi^{1,+} \ , \ \partial_\ell \chi^y = ... - 4\eta^y \psi^{1,-} \ , \ \partial_\ell \chi^z = ... + 4\eta^z \psi^{1,+} \tag{C14}$$

$$\partial_\ell \psi^{x,+} = ... - 2\eta^z \varphi^{y,+} 1_n - 6\eta^y \varphi^{z,+} 1_n \tag{C15}$$

$$\partial_\ell \psi^y = ... - 4\eta^z \varphi^{x,-} 1_n + 4\eta^x \varphi^{z,-} 1_n \tag{C16}$$

$$\partial_\ell \psi^{z,+} = ... + 2\eta^x \varphi^{y,+} 1_n + 6\eta^y \varphi^{x,+} 1_n \tag{C17}$$

$$\partial_\ell \psi^{x,-} = ... - 6\eta^z \varphi^{y,-} 1_n - 4\eta^y \varphi^{z,-} 1_n \tag{C18}$$

$$\partial_\ell \psi^{z,-} = ... + 6\eta^x \varphi^{y,-} 1_n + 4\eta^y \varphi^{x,-} 1_n \tag{C19}$$

The flow equations for the new parameters of $\sigma_z^{new,3}$ yield:

$$\partial_\ell \psi^{1,+} = 6\eta^z \varphi^{z,+} + 2\eta^y \varphi^{y,+} + 6\eta^x \varphi^{x,+} \tag{C20}$$

$$\partial_\ell \psi^{1,-} = 2\eta^z \varphi^{z,-} + 6\eta^y \varphi^{y,-} + 2\eta^x \varphi^{x,-} \tag{C21}$$

$$\partial_\ell \varphi^{x,+} = -2\eta^y \psi^{z,+} - 2\eta^{0,y} \varphi^{z,+} \tag{C22}$$

$$\partial_\ell \varphi^{y,+} = 2\eta^z \psi^{x,-} - 2\eta^x \psi^{z,-} \tag{C23}$$

$$\partial_\ell \varphi^{z,+} = 2\eta^y \psi^{z,+} + 2\eta^{0,y} \varphi^{x,+} \tag{C24}$$

$$\partial_\ell \varphi^{x,-} = 2\eta^z \psi^y - 2\eta^y \psi^{z,-} - 2\eta^{0,y} \varphi^{z,-} \tag{C25}$$

$$\partial_\ell \varphi^{y,-} = 2\eta^z \psi^{x,+} - 2\eta^x \psi^{z,+} \tag{C26}$$

$$\partial_\ell \varphi^{z,-} = -2\eta^x \psi^y + 2\eta^y \psi^{x,-} + 2\eta^{0,y} \varphi^{x,-} \tag{C27}$$

APPENDIX D: RABI MODEL IN PERTURBATION THEORY

In this appendix we will treat the Rabi Hamiltonian in perturbation theory. We want to start from the exactly solvable Jaynes-Cummings Hamiltonian which is obtained from the symmetric Rabi Hamiltonian with no bias by applying the rotating wave approximation[19]. This approximation neglects coupling or transition terms which are energetically unlikely.

It is useful to write the Hamiltonian in a basis where σ_x is diagonal. The Rabi Hamiltonian shall thus be given by

$$H = \sum_{i=0,1} \epsilon_i c_i^\dagger c_i + \omega_0 b^\dagger b + \lambda b c_1^\dagger c_0 + \lambda b^\dagger c_0^\dagger c_1 + \lambda' b^\dagger c_1^\dagger c_0 + \lambda' b c_0^\dagger c_1 \quad . \tag{D1}$$

The operators $c_i^{(\dagger)}$ and $b^{(\dagger)}$ obey the canonical anti-commutation and commutation relations respectively. We identify the Rabi Hamiltonian given in Eq. (1) by setting $\epsilon_1 - \epsilon_0 = \Delta_0$ and $\lambda = \lambda' = 2\lambda_0$ and the zero external bias.

The Jaynes-Cummings Hamiltonian is obtained by setting $\lambda' = 0$ in Eq. (D1). We want to treat the so called off-shell processes, characterized by λ', within a systematic perturbation approach. One way to do so is to consider the Hamiltonian in the basis $\{|0;2n\rangle|1;2n+1\rangle\}$ and $\{|0;2n+1\rangle,|1;2n\rangle\}$ where the first quantum number resembles the fermionic state and the second quantum number the bosonic state. Since the Hamiltonian is symmetric with respect to parity the two sets decouple and in the following we will only consider the first set.

In the above basis, the Hamiltonian is tridiagonal and we define the n-dependent matrices

$$D^{\text{on}}(n) \equiv \begin{pmatrix} \epsilon_1 + 2n\omega_0 & \sqrt{2n+1}\lambda \\ \sqrt{2n+1}\lambda & D^{\text{off}}(n+1) \end{pmatrix} \quad ,$$

$$D^{\text{off}}(n+1) \equiv \begin{pmatrix} \epsilon_0 + (2n+1)\omega_0 & \sqrt{2n+2}\lambda' \\ \sqrt{2n+2}\lambda' & D^{\text{on}}(n+1) \end{pmatrix} \quad . \tag{D2}$$

The determinants can formally be evaluated to yield

$$\det D^{\text{on}}(n) = (\epsilon_1 + 2n\omega_0)\det D^{\text{off}}(n+1) - (2n+1)\lambda^2 \det D^{\text{on}}(n+1) \tag{D3}$$

$$\det D^{\text{off}}(n+1) = (\epsilon_0 + (2n+1)\omega_0)\det D^{\text{on}}(n+1) - (2n+2)\lambda'^2 \det D^{\text{off}}(n+2) \quad .$$

The matrix $D^{\text{on}}(0)$ resembles the representation of the Rabi Hamiltonian in the above basis. To determine the eigenvalue μ of the matrix up to $O(\lambda'^2)$ we iterate Eq. (D3) starting with $D^{\text{on}}(0)$:

$$\det(D^{\text{on}}(0) - \mu) \rightarrow \left[(\epsilon_1 - \mu)(\epsilon_0 + \omega_0 - \mu) - \lambda^2\right]$$
$$\times \left[(\epsilon_1 + 2\omega_0 - \mu)(\epsilon_0 + 3\omega_0 - \mu) - 3\lambda^2\right]\det(D^{\text{on}}(2) - \mu) \tag{D4}$$
$$-(\epsilon_1 - \mu)2\lambda'^2(\epsilon_0 + 3\omega_0 - \mu)\det(D^{\text{on}}(2) - \mu) = 0$$

For the eigenvalues we make the ansatz $\mu = \mu^{(0)} + \lambda'^2 \mu^{(1)}$. There is no linear term in λ' since the spectrum of H may not depend on the phase of the coupling constant.

We now order the eigenvalues as follows: The lowest eigenvalues of order $O(\lambda'^0)$, $\mu_{0,\pm}^{(0)}$, are determined by setting the first factor on the right hand side of Eq. (D4) zero. We obtain the well-known Jaynes-Cummings result $\mu_{0,\pm}^{(0)} =$

$\epsilon_0 + \omega_0 - (\bar{\Delta} \mp R_0)/2$ with the detuning $\bar{\Delta} \equiv (\epsilon_1 - \epsilon_0) - \omega_0$ and the zeroth Rabi frequency $R_0^2 = \bar{\Delta}^2 + 4\lambda^2$. The first correction to $\mu_{0,\pm}^{(0)}$ then yields

$$\mu_{0,\pm}^{(1)} = \frac{1}{\mp R_0} \frac{\bar{\Delta}\omega_0 \pm R_0\omega_0 - \lambda^2}{2\omega_0^2 \mp R_0\omega_0 - \lambda^2} \quad . \tag{D5}$$

The result agrees with the perturbative result in the limit $\lambda = \lambda' \ll \bar{\Delta}$.

Generally, setting the nth factor of the first line on the right hand side of Eq. (D4) zero the nth eigenvalues yield $\mu_{n,\pm}^{(0)} = \epsilon_0 + (2n+1)\omega_0 - (\bar{\Delta} \mp R_n)/2$ with $R_n^2 = \bar{\Delta}^2 + 4(2n+1)\lambda^2$. The first correction to $\mu_{n,\pm}^{(0)}$ is given by

$$\mu_{n,\pm}^{(1)} = \frac{1}{\mp R_n}\left[(n+1)\frac{\bar{\Delta}\omega_0 \pm R_n\omega_0 - \lambda^2}{2\omega_0^2 \mp R_n\omega_0 - (n+1)\lambda^2} + n\frac{\bar{\Delta}\omega_0 \mp R_n\omega_0 - \lambda^2}{2\omega_0^2 \pm R_n\omega_0 - (n-1)\lambda^2}\right] \quad . \tag{D6}$$

The perturbative approach breaks down when degenerated states are involved. This is indicated by the poles in the energy corrections $\mu_{n,\pm}^{(1)}$. Setting the denominator of $\mu_{0,\pm}^{(1)}$ zero, one obtains for the tunnel-matrix element $\Delta_0 = \omega_0 + \sqrt{(2\omega_0^2 - \lambda^2)^2 - 4\omega_0^2\lambda^2}/\omega_0$. Inserting the parameters used for Fig. 8, we obtain $\Delta_0 \approx 2.87$. This value approximately agrees with the value of Δ_0 where the second spike of h_z in Figure 8 is seen.

APPENDIX E: NORMAL ORDERING

In this appendix we want to summarize basic relations concerning normal ordering. This summary is based on unpublished notes by Wegner of the year 2000 in which he presents a general formalism for normal ordering of classical and quantum fields with respect to a bilinear Hamiltonian[26]. We will restrain ourselves to the normal ordering of bosonic quantum fields.

Let b_k be any linear combination of Bose creation and annihilation operators. The matrix G shall describe the correlations of the operators b for a Hamiltonian H bilinear in the creation and annihilation operators: $\langle b_k b_l \rangle = G_{kl}$. The commutator is given by $[b_k, b_l] = G_{kl} - G_{lk}$. Normal ordering of an operator A with respect to the Hamiltonian H is now defined by:

$$: 1 := 1 \tag{E1}$$

$$: \alpha A(b) + \beta B(b) := \alpha : A(b) : + \beta : B(b) : \tag{E2}$$

$$b_k : A(b) := : b_k A(b) : + \sum_l G_{kl} : \frac{\partial A(b)}{\partial b_k} : \tag{E3}$$

The product of m operators b_{k_i} with $i = 1..m$ is now obtained by iterating the third equation. One obtains

$$b_{k_1}b_{k_2}...b_{k_m} =: (b_{k_1} + \sum_{l_1} G_{k_1,l_1}\frac{\partial}{\partial b_{l_1}})(b_{k_2} + \sum_{l_2} G_{k_2,l_2}\frac{\partial}{\partial b_{l_2}})...b_{k_m} : \quad , \tag{E4}$$

which can also be written as

$$b_{k_1}b_{k_2}...b_{k_m} =: \exp(\sum_{kl} G_{kl}\frac{\partial^2}{\partial b_k^{left}\partial b_l^{right}})b_{k_1}b_{k_2}...b_{k_m} : \quad . \tag{E5}$$

This is Wick's first theorem[27]. The superscripts ^{left} and ^{right} indicate that we always pick a pair of factors b and perform the derivative $\partial/\partial b_k$ on the left factor and the derivative $\partial/\partial b_l$ on the right factor, so that the factor G_{kl} depends on the sequence of the operators.

Similarly one obtains

$$: b_{k_1}b_{k_2}...b_{k_m} := \exp(-\sum_{kl} G_{kl}\frac{\partial^2}{\partial b_k^{left}\partial b_l^{right}})b_{k_1}b_{k_2}...b_{k_m} \quad . \tag{E6}$$

The formula for the product of two normal ordered operators is given by

$$: A(b) :: B(b) := : \exp(\sum_{kl} G_{kl}\frac{\partial^2}{\partial b_k\partial a_l})A(b)B(a) : |_{a=b} \quad . \tag{E7}$$

This is Wicks's second theorem.

One can now show that under normal ordering the commutative law holds: $: ABCD :=: ACBD :$. This is rule C of Wick.

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